

August 1997

ISSN 0301-0104

Chemical Physics

**A journal devoted to experimental and theoretical research
involving problems of both a chemical and a physical nature**

MASTER INDEX

VOLUMES 211-220

NOVEMBER 1996 – AUGUST 1997

Editors

ROBIN M. HOCHSTRASSER/G. LUDWIG HOFACKER

NORTH-HOLLAND

Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER
Department of Chemistry, University of Pennsylvania,
Philadelphia, PA 19104-6323, USA
FAX: 1-215-8980590
E-mail: hochstra@a.chem.upenn.edu

G. LUDWIG HOFACKER
Lehrstuhl für Theoretische Chemie, Technische Universität
München,
Lichtenbergstrasse 4, 85747 Garching, Germany
FAX: 49-89-28913622
E-mail: hofacker@theochem.tu-muenchen.de

ASSOCIATE EDITORS

DAVID CHANDLER, Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA. FAX: 1-510-6428369;
E-mail: chandler@cchem.berkeley.edu

H. PETER TROMMSDORFF, Laboratoire de Spectrométrie Physique, Université Joseph-Fourier Grenoble I, B.P. 87, 38402 Saint-Martin-d'Hères Cedex, France. FAX: 33-76-514544; E-mail: trommsdo@spectro.grenet.fr

ADVISORY EDITORIAL BOARD

Australia

D.J. EVANS, Canberra
N.S. HUSH, Sydney
R.O. WATTS, Parkville

Canada

R.J.D. MILLER, Toronto

Denmark

G.D. BILLING, Copenhagen

France

S. LEACH, Orsay
D. MARKOVITSI, Gif-sur-Yvette
J.L. MARTIN, Palaiseau
M. ORRIT, Talence

Germany

H. BÄSSLER, Marburg
B. DICK, Regensburg
S.F. FISCHER, Garching
H. GRABERT, Freiburg
D. HAARER, Bayreuth
P. HÄNGGI, Augsburg
W. LORENZ, Leipzig
D. MENZEL, Garching
M. PARRINELLO, Stuttgart
E.W. SCHLAG, Garching
W. ZINTH, Munich

Hungary

P. ORMOS, Szeged

Israel

R.B. GERBER, Jerusalem
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
E. POLLAK, Rehovot

Italy

G. CICCOTTI, Rome

Japan

H. HAMAGUCHI, Tokyo
M. ITO, Okazaki
T. KITAGAWA, Okazaki
T. KOBAYASHI, Tokyo
K. YOSHIHARA, Okazaki

The Netherlands

D. FRENKEL, Amsterdam

Russian Federation

V.S. LETOKHOV, Moscow

Sweden

R. RIGLER, Stockholm

Switzerland

H. FISCHER, Zurich
S. LEUTWYLER, Bern

Taiwan

Y.T. LEE, Taipei

United Kingdom

A.D. BUCKINGHAM, Cambridge
D.A. KING, Cambridge
P.A. MADDEN, Oxford
J.P. SIMONS, Oxford

USA

A.C. ALBRECHT, Ithaca, NY
P. ALIVISATOS, Berkeley, CA
V.A. APKARIAN, Irvine, CA
P.F. BARBARA, Minneapolis, MN
R. BERSOHN, New York, NY
S.G. BOXER, Stanford, CA
S.T. CEYER, Cambridge, MA
K.A. DILL, San Francisco, CA
W.A. EATON, Bethesda, MD
M.D. FAYER, Stanford, CA
G.R. FLEMING, Chicago, IL
G. FLYNN, New York, NY
R.A. FRIESNER, New York, NY
M. KLEIN, Philadelphia, PA

USA (continued)

W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
D.M. NEUMARK, Berkeley, CA
M.D. NEWTON, Upton, NY
C.S. PARMENTER, Bloomington, IN
M.A. RATNER, Evanston, IL
G.W. ROBINSON, Lubbock, TX
G.J. SMALL, Ames, IA
J.C. TULLY, New Haven, CT
J.D. WEEKS, College Park, MD
K.B. WHALEY, Berkeley, CA
P.G. WOLYNES, Urbana, IL
R.N. ZARE, Stanford, CA
A.H. ZEWEIL, Pasadena, CA

AIMS AND SCOPE

Chemical Physics publishes experimental and theoretical papers on all aspects of chemical physics. Experimental papers are brought into relation with theory and theoretical papers demonstrate their relation to present or future experiments. More specifically, subject matter in the fields of spectroscopy and molecular structure, interacting systems, relaxation phenomena, fundamental problems in molecular reactivity, molecular quantum theory and statistical mechanics constitute the main areas of interest for this journal. In addition to regular issues, *Chemical Physics* publishes thematic issues containing invited articles by specialists in the relevant field.

Chemical Physics

EDITORS

ROBIN M. HOCHSTRASSER

Department of Chemistry, University of Pennsylvania,

Philadelphia, PA 19104-6323, USA

FAX: 1-215-8980590

E-mail: hochstra@chem.upenn.edu

G. LUDWIG HOFACKER

Lehrstuhl für Theoretische Chemie, Technische Universität München,

Lichtenbergstrasse 4, 85747 Garching, Germany

FAX: 49-89-28913622

E-mail: hofacker@theochem.tu-muenchen.de

ASSOCIATE EDITORS

DAVID CHANDLER, Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA. FAX: 1-510-6428369; E-mail:

chandler@cchem.berkeley.edu

H. PETER TROMMSDORFF, Laboratoire de Spectrométrie Physique, Université Joseph-Fourier Grenoble I, B.P. 87, 38402 Saint-Martin-d'Hères Cedex,

France. FAX: 33-76-514544; E-mail: trommsdo@spectro.grenet.fr

ADVISORY EDITORIAL BOARD

Australia

D.J. EVANS, Canberra

N.S. HUSH, Sydney

R.O. WATTS, Parkville

Canada

R.J.D. MILLER, Toronto

Denmark

G.D. BILLING, Copenhagen

France

S. LEACH, Orsay

D. MARKOVITSI, Gif-sur-Yvette

J.L. MARTIN, Palaiseau

M. ORRIT, Talence

Germany

H. BÄSSLER, Marburg

B. DICK, Regensburg

S.F. FISCHER, Garching

H. GRABERT, Freiburg

D. HAARER, Bayreuth

P. HÄNGGI, Augsburg

W. LORENZ, Leipzig

D. MENZEL, Garching

M. PARRINELLO, Stuttgart

E.W. SCHLAG, Garching

W. ZINTH, Munich

Hungary

P. ORMOS, Szeged

Israel

R.B. GERBER, Jerusalem

J. JORTNER, Tel Aviv

R.D. LEVINE, Jerusalem

E. POLLAK, Rehovot

Italy

G. CICCOTTI, Rome

Japan

H. HAMAGUCHI, Tokyo

M. ITO, Okazaki

T. KITAGAWA, Okazaki

T. KOBAYASHI, Tokyo

K. YOSHIHARA, Okazaki

The Netherlands

D. FRENKEL, Amsterdam

Russian Federation

V.S. LETOKHOV, Moscow

Sweden

R. RIGLER, Stockholm

Switzerland

H. FISCHER, Zurich

S. LEUTWYLER, Bern

Taiwan

Y.T. LEE, Taipei

United Kingdom

A.D. BUCKINGHAM, Cambridge

D.A. KING, Cambridge

P.A. MADDEN, Oxford

J.P. SIMONS, Oxford

USA

A.C. ALBRECHT, Ithaca, NY

P. ALIVISATOS, Berkeley, CA

V.A. APKARIAN, Irvine, CA

P.F. BARBARA, Minneapolis, MN

R. BERSOHN, New York, NY

S.G. BOXER, Stanford, CA

S.T. CEYER, Cambridge, MA

K.A. DILL, San Francisco, CA

W.A. EATON, Bethesda, MD

M.D. FAYER, Stanford, CA

G.R. FLEMING, Chicago, IL

G. FLYNN, New York, NY

R.A. FRIESNER, New York, NY

M. KLEIN, Philadelphia, PA

USA (continued)

W.C. LINEBERGER, Boulder, CO

D.S. McCLURE, Princeton, NJ

D.M. NEUMARK, Berkeley, CA

M.D. NEWTON, Upton, NY

C.S. PARMENTER, Bloomington, IN

M.A. RATNER, Evanston, IL

G.W. ROBINSON, Lubbock, TX

G.J. SMALL, Ames, IA

J.C. TULLY, New Haven, CT

J.D. WEEKS, College Park, MD

K.B. WHALEY, Berkeley, CA

P.G. WOLYNES, Urbana, IL

R.N. ZARE, Stanford, CA

A.H. ZEWEIL, Pasadena, CA

Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs.

CHEMICAL PHYSICS

Editors

ROBIN M. HOCHSTRASSER, Philadelphia

G. LUDWIG HOFACKER, Munich

Associate Editors

DAVID CHANDLER, Berkeley

H. PETER TROMMSDORFF, Saint-Martin-d'Hères

MASTER INDEX

VOLUMES 211-220

NOVEMBER 1996 – AUGUST 1997



ELSEVIER

Amsterdam – Lausanne – New York – Oxford – Shannon – Tokyo

This journal and the individual contributions contained in it are protected by the copyright of Elsevier Science B.V., and the following terms and conditions apply to their use:

Photocopying

Single photocopies of single articles may be made for personal use as allowed by national copyright laws. Permission of the Publisher and payment of a fee is required for all other photocopying, including multiple or systematic copying, copying for advertising or promotional purposes, resale, and all forms of document delivery. Special rates are available for educational institutions that wish to make photocopies for non-profit educational classroom use.

In the USA, users may clear permissions and make payment through the Copyright Clearance Center Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In the UK, users may clear permissions and make payment through the Copyright Licensing Agency Rapid Clearance Service (CLARCS), 90 Tottenham Court Road, London W1P 0LP, UK. In other countries where a local copyright clearance centre exists, please contact it for information on required permissions and payments.

Derivative Works

Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions. Permission of the Publisher is required for resale or distribution outside the institution.

Permission of the Publisher is required for all other derivative works, including compilations and translations.

Electronic Storage

Permission of the Publisher is required to store electronically any material contained in this journal, including any article or part of an article. Contact the Publisher at the address indicated.

Except as outlined above, no part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without prior written permission of the Publisher.

Disclaimers

No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein.

Although all advertising material is expected to conform to ethical (medical) standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Elsevier Science B.V.
Tel: (+31-20)4852-800 Fax: (+31-20)4852-775 E-mail: e.hovens@elsevier.nl

Postal Address

Chemical Physics
Elsevier Science B.V.
P.O. Box 2759
1000 CT Amsterdam
The Netherlands

Courier Service Address

Chemical Physics
Elsevier Science B.V.
Sara Burgerhartstraat 25
1055 KV Amsterdam
The Netherlands

© The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper)

Printed in the Netherlands.

Contents

Author index to volumes 211-220	1	Field emission and field ionization	64
Subject index to volumes 211-220	37	Measurement of macroscopic variables	64
METHODS	37	OBJECTS	64
<i>Theoretical</i>	37	<i>Bulk systems</i>	64
Group theory and algebras	37	Gases	64
Classical mechanics	37	Supersonic beams	66
Many body and quasiparticle approaches	38	Liquids neat	66
Coupling schemes and perturbative treatments	38	Liquid mixtures and solutions	66
Relativistic quantum mechanics	39	Crystals	68
Transport quantum mechanics	39	neat	69
Equilibrium statistical mechanics	40	mixed	69
Statistical mechanics of stationary states	40	Glasses	69
Non-equilibrium thermodynamic and hydrodynamic theories	41	Liquid crystals	70
Ab initio schemes for stationary properties	41	Polymers	70
Computational and simulation methods	44	Semiconductors	70
Molecular dynamics and scattering theory	48	Metals and alloys	70
<i>Experimental</i>	50	Thin films	71
Magnetic resonances	50	Surfaces	71
Cyclotron resonance	51	Low-dimensional materials	71
Microwave spectroscopy	51	Dielectrics	71
Infrared spectroscopy	51	Plasmas	71
Raman spectroscopy	52	Biological systems	72
Visible and UV spectroscopy	52	<i>Microscopic systems</i>	72
Fluorescence spectroscopy	55	Atoms	72
Photoelectron and Auger spectroscopy	57	Molecules (neutral and ionic)	73
X-ray spectroscopy	57	diatomic	75
Electron impact spectroscopy	57	small polyatomics	77
Laser methods	58	aromatics	79
Picosecond spectroscopy	59	other large	81
Non-linear optical spectroscopy	59	polymeric and biological	81
Synchrotron spectroscopies	60	Molecular aggregates	82
Coherent optical spectroscopy	60	dimers	83
Optical pumping	60	van der Waals molecules	83
Multiple resonance spectroscopy	60	clusters	84
Optoacoustic spectroscopy	60	complexes	85
Atomic and molecular beam techniques	61	Free radicals (including hydronium and muonium)	85
Time-resolved experiments	61	Quasiparticles (including excitons)	86
Mass spectrometry	63	Defects and impurities	86
Radiolysis	63	Ions and charge carriers	86
Mössbauer spectroscopy	63	PHENOMENA	87
X-ray, electron and neutron diffraction	63	Molecular structure	87
Neutron scattering	63	Vibrations and rotations of molecules	88
Light scattering	64		

Electronic structure and states	90	Reactions (including dissociation)	102
Electric and magnetic properties	93	gas phase	102
Spin splittings	94	condensed phase	103
Optical activity	94	photochemical	104
Molecular interactions	94	Tunnelling	105
Spectral bandshapes and intensities	95	Electron transfer	105
Coupling of electronic and nuclear motion	96	Positron annihilation	107
Energy transfer processes	97	Ionization (including Rydberg states)	107
Molecular photophysical processes	98	Molecular motion (including diffusive)	108
Intramolecular dynamics	99	Isotopic effects	109
radiationless transitions	99	Fluctuations and noise	109
vibrational energy redistribution		Collective motion and excitations	109
(including vibrational dissociation)	99	Surface effects and catalysis	109
Luminescence spectra, yields and lifetimes	100	Thermodynamic and transport properties	110
Coherence loss processes	100	Structure of solids and liquids	110
Non-linear responses (including optical)	101	Critical phenomena	111
Multiphoton phenomena	101	Phase transitions	111



ELSEVIER

Chemical Physics 211–220 (1997) 1–35

Chemical
Physics

Author index to volume 211–220

- Abraham, E., J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière, Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry 214 (1997) 409
- Abraham, E., J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière, Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push-pull diphenyl-polyenes: evidence for 'loose' complex and 'bimer' species 219 (1997) 73
- Abramczyk, H., see Kolodziejski, M. 213 (1996) 341
- Adamowicz, L., see Sobolewski, A.L. 213 (1996) 193
- Adhikari, S., see Sarkar, P. 215 (1997) 309
- Adrian, F.J., Spin-orbit effects in fullerenes 211 (1996) 73
- Agmon, N. and G.M. Sastry, A temperature-dependent effective potential explains CO binding to myoglobin 212 (1996) 207
- Ågren, H., see Minaev, B.F. 220 (1997) 79
- Aguilar, M.A., see Contador, J.C. 214 (1997) 113
- Ahmed, M., C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk, Fluorescence excitation spectroscopy of some haloethenes, $\text{CF}_2=\text{CXY}$ ($\text{XY} \equiv \text{FCl}, \text{Cl}_2, \text{FH}$), excited in the vacuum ultraviolet (70–180 nm) 219 (1997) 333
- Alikacem, A., see Boudjarane, K. 211 (1996) 393
- Alikhani, M.E., see Tremblay, B. 218 (1997) 37
- Allers, S.J.R., see Svendsen, C. 215 (1997) 89
- Allonas, X. and P. Jacques, Factors affecting adiabaticity in bimolecular photoinduced electron transfer reaction between anthracene derivatives and organic donors 215 (1997) 371
- Aloisio, S. and J.S. Francisco, Ab initio study of the structure, vibrational spectra and binding energy of $\text{HCl}-\text{ClO}$ and Cl_2-ClO complexes 219 (1997) 201
- Alonso, J.L., F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler, Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran-argon van der Waals complex 218 (1997) 267
- Althorpe, S.C., D.J. Kouri, D.K. Hoffman and N. Moiseyev, A time-independent wavepacket approach to the (t, t') -method for treating time-dependent Hamiltonian systems 217 (1997) 289
- Amaya-Tapia, A., see Martinez, H. 211 (1996) 299
- André, J.-M., see Jacquemin, D. 213 (1996) 217
- Andrés, J., see Camargo, A.C. 212 (1996) 381
- Andrés, J.L., see Luis, J.M. 217 (1997) 29
- Andrews, D.L. and I.D. Hands, Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors 213 (1996) 277
- Ankerhold, U., B. Esser and F. von Busch, Ionization and fragmentation of OCS and CS_2 after photoexcitation around the sulfur 2p edge 220 (1997) 393

- Antoine, R., see Dugourd, Ph. 218 (1997) 163
- Apkarian, V.A., see Logan, D. 217 (1997) 99
- Apkarian, V.A., see Grigorenko, B.L. 219 (1997) 161
- Apps, C.J., see Ahmed, M. 219 (1997) 333
- Aquilanti, V., S. Cavalli and C. Coletti, The d -dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals and alternative Sturmian basis sets 214 (1997) 1
- Arabei, S.M., S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup, Sol-gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis 216 (1997) 163
- Aratono, Y., see Kumada, T. 212 (1996) 177
- Asawakun, P., see Sagarik, K. 219 (1997) 173
- Atkinson, G.H., see Ujj, L. 212 (1996) 421
- Atkinson, G.H., see Ujj, L. 217 (1997) 115
- Au, J.W., G. Cooper and C.E. Brion, Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3 : absolute oscillator strengths and dipole-induced breakdown pathways 215 (1997) 397
- Au, J.W. and C.E. Brion, Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions 218 (1997) 87
- Au, J.W. and C.E. Brion, Absolute oscillator strengths for the valence-shell photoabsorption (2-200 eV) and the molecular and dissociative photoionization (11-80 eV) of nitrogen dioxide 218 (1997) 109
- Azumi, T., see Tarasov, V.F. 212 (1996) 353
- Bach, S.B.H., see Canty, J.F. 216 (1997) 81
- Bacis, R., see Cerny, D. 216 (1997) 207
- Backhaus, P. and B. Schmidt, Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury 217 (1997) 131
- Baddour-Hadjean, R., see Fillaux, F. 216 (1997) 281
- Bagnich, S.A., Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution 214 (1997) 351
- Bagnich, S.A., The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses 218 (1997) 277
- Bahou, M., L. Schriver-Mazzuoli, A. Schriver and P. Chaquin, Structure and selective visible photodissociation of the $\text{O}_3:\text{Br}_2$ and $\text{O}_3:\text{BrCl}$ complexes: an infrared matrix isolation and ab initio study 216 (1997) 105
- Bakó, I., J.C. Dore and D.W. Huxley, Orientational correlations in liquid carbon tetrabromide: a neutron diffraction and RMC study 216 (1997) 119
- Ball, D.W., see Canty, J.F. 216 (1997) 81
- Baltzer, P., see Eland, J.H.D. 212 (1996) 457
- Baltzer, P., see Holland, D.M.P. 219 (1997) 91
- Baraille, I., see Habas, M.-P. 219 (1997) 63
- Baranowski, A., K. Jerie and J. Gliński, Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures 214 (1997) 143
- Barkai, E. and V. Fleurov, Dissipation and fluctuation for a randomly kicked particle: Normal and anomalous diffusion 212 (1996) 69
- Bässler, H., see Tak, Y.-H. 212 (1996) 471
- Baumann, W., see Reis, H. 214 (1997) 383
- Baumgärtel, H., see Biehl, H. 214 (1997) 367
- Baumgärtel, H., see Eisenhardt, C.G. 216 (1997) 427

- Baumgärtel, H., see Locht, R. 220 (1997) 207
- Baumgärtel, H., see Locht, R. 220 (1997) 217
- Baumgarten, M., see Zhang, J. 214 (1997) 291
- Bauschlicher Jr., C.W., The dissociation energies of FeF, FeCl, and FeBr and their positive ions 211 (1996) 163
- Bazhenov, A.V., see Kveder, V.V. 216 (1997) 407
- Beckmann, S., see Steybe, F. 219 (1997) 317
- Beghin, A. and T. Stoecklin, The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory 215 (1997) 261
- Beijerinck, H.C.W., see Vredendregt, E.J.D. 216 (1997) 259
- Beijerinck, H.C.W., see Vredendregt, E.J.D. 216 (1997) 273
- Belchior, J.C. and J.P. Braga, A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions 213 (1996) 303
- Belikov, A.E., R.G. Sharafutdinov and A.V. Storozhev, Rotational relaxation of nitrogen in helium 213 (1996) 319
- Belikov, A.E., Rotational and vibrational excitation of the N_2^+ (B) state in a He + N_2 electron-beam plasma 215 (1997) 97
- Belinsky, M.I., Double exchange in distorted trimeric mixed-valence clusters 215 (1997) 7
- Bell, I.M., see Torii, H. 216 (1997) 67
- Beltrán, A., see Camargo, A.C. 212 (1996) 381
- Belyaev, A.K. and A.S. Tiukanov, Diatomics-in-molecules study of the ground and excited states of H_3^- 220 (1997) 43
- Bendazzoli, G.L., S. Evangelisti and F. Passarini, Is He H^- a stable system? 215 (1997) 217
- Bender, S., see Franke, R. 216 (1997) 243
- Benderskii, V.A., E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff, Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach 219 (1997) 119
- Benderskii, V.A., E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff, Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states 219 (1997) 143
- Benetis, N.P., see Salih, N.A. 212 (1996) 409
- Bensasson, R.V., T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt, Spectroscopy and photophysics of $C_{60}H_{18}$ and $C_{60}H_{36}$ 215 (1997) 111
- Bergmann, F., see Lorenz, W. 215 (1997) 139
- Bergmann, F., M. Handschuh and W. Lorenz, Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions 215 (1997) 157
- Berlin, Y.A., A.L. Burin and S.F. Fischer, Phenomenological model for reaction kinetics coupled to a relaxing environment 220 (1997) 25
- Berlin, Yu.A., Irreversible random transition theory as applied to rate processes in condensed media: Transient effects of constrained configuration rearrangements in complex systems 212 (1996) 29
- Bernardes, E.S., Y.M.M. Hornos and J.E.M. Hornos, Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF) 213 (1996) 17
- Berning, A., see Leininger, T. 217 (1997) 19
- Bertault, M., see Even, J. 213 (1996) 357
- Bertault, M., see Delcourt, O. 215 (1997) 51

- Bessis, D., see Felfli, Z. 211 (1996) 325
- Bettinelli, M., see Capobianco, J.A. 214 (1997) 329
- Bhattacharyya, S.P., see Sarkar, P. 215 (1997) 309
- Biehl, H., K.J. Boyle, D.M. Smith and R.P. Tuckett, The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF_3X^+ ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) ions 214 (1997) 357
- Biehl, H., K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims, Vacuum-UV fluorescence spectroscopy of CF_3X ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) in the range 10–30 eV 214 (1997) 367
- Biertümpel, I. and H.-H. Schmidtke, Evaluation of luminescence decay measurements probed on pure and doped Pt(IV) hexahalogeno complexes I. Exponential rise time and decay curves applying various statistical tests 215 (1997) 271
- Bieser, G., see Lossau, H. 213 (1996) 1
- Billing, G.D., see Gross, A. 217 (1997) 1
- Bizot, H., see Leroux, B. 216 (1997) 349
- Bizzarri, A.R., see Rocchi, C. 214 (1997) 261
- Blake, A.J., see Jones, A.L. 211 (1996) 291
- Bleyer, A., see Tak, Y.-H. 212 (1996) 471
- Bodenbinder, M., see Tyczkowski, G. 215 (1997) 379
- Boeglin, A., see Klein, G. 215 (1997) 131
- Böhm, M.C., see Schmidt, R.G. 215 (1997) 207
- Boilot, J.P., see Kulikov, S.G. 216 (1997) 147
- Boilot, J.P., see Brunel, M. 218 (1997) 301
- Bojarski, P. and L. Kułak, Forward and reverse excitation energy transport in concentrated two-component systems 220 (1997) 323
- Boldyrev, S.I., see Coropceanu, V.P. 219 (1997) 1
- Bolognesi, P., see Yench, A.J. 216 (1997) 227
- Bolvin, H., The Neel point for spin-transition systems: toward a two-step transition 211 (1996) 101
- Bondybey, V.E., see Caspary, N. 220 (1997) 241
- Borchert, I., see Ruth, C. 213 (1996) 454
- Börjesson, L.E.B. and S. Nordholm, A partially ergodic multiple encounter theory of collisional energy transfer 212 (1996) 393
- Borsenberger, P.M., see Sinicropi, J.A. 218 (1997) 331
- Boudjarane, K., A. Alikacem and M. Larzillière, Fast-ion beam laser spectroscopy of $^{14}\text{N}_2^+$ and $^{15}\text{N}_2^+$: high-resolution study of the (1, 2) band of the $\text{B } ^2\Sigma_u^+ - \text{X } ^2\Sigma_g^+$ system 211 (1996) 393
- Boughton, J.W., S. Kristyan and M.C. Lin, Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations 214 (1997) 219
- Boukheddaden, K., see Varret, F. 212 (1996) 487
- Boukheddaden, K. and F. Varret, Vibronic theory of electric hysteresis in “bistable” mixed-valence molecular salts 216 (1997) 373
- Bouteiller, Y., see Coussan, S. 219 (1997) 221
- Boyle, K.J., see Biehl, H. 214 (1997) 357
- Boyle, K.J., see Biehl, H. 214 (1997) 367
- Brady, J.W., see Leroux, B. 216 (1997) 349
- Braga, M., Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α, ω -diethynyl[n]staffanes ($n = 1-5$) 213 (1996) 159
- Braga, J.P., see Belchior, J.C. 213 (1996) 303
- Braidwood, S., see Zheng, Y. 212 (1996) 269

- Bramwell, M.J., see Ahmed, M. 219 (1997) 333
- Brazgun, F.F., V.A. Nadtochenko, I.V. Rubtsov and L.V. Lukin, Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique 211 (1996) 469
- Brickmann, J., see Schmidt, R.G. 215 (1997) 207
- Brickmann, J., see Gudowska-Nowak, E. 220 (1997) 125
- Brint, R.P., see Ruth, A.A. 217 (1997) 83
- Brion, C.E., see Zheng, Y. 212 (1996) 269
- Brion, C.E., see Rolke, J. 215 (1997) 191
- Brion, C.E., see Au, J.W. 215 (1997) 397
- Brion, C.E., see Au, J.W. 218 (1997) 87
- Brion, C.E., see Au, J.W. 218 (1997) 109
- Brion, C.E., see Olney, T.N. 218 (1997) 127
- Broo, A. and A. Holmén, Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives 211 (1996) 147
- Broyer, M., see Dugourd, Ph. 218 (1997) 163
- Brumer, P., see Shapiro, M. 217 (1997) 325
- Brun, A., see Brunel, M. 218 (1997) 301
- Brunel, M., F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun, Reverse saturable absorption in palladium and zinc tetraphenyltetraenzoporphyrin doped xerogels 218 (1997) 301
- Brunger, M.J., see Zheng, Y. 212 (1996) 269
- Buijsse, B., see Wouters, E.R. 218 (1997) 309
- Buonomo, E., F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal, A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster 218 (1997) 71
- Burin, A.L., see Berlin, Y.A. 220 (1997) 25
- Burrows, H.D., see Ferreira Marques, M.F. 220 (1997) 233
- Burshtein, A.I. and P.A. Frantsuzov, Remote ionization and recombination through the multichannel electron transfer 212 (1996) 137
- Burton, G.R., see Olney, T.N. 218 (1997) 127
- Büttner, H.G., G.J. Kearley and B. Frick, Tunnelling of the one-dimensional rotor NH_3D^+ in the NH_4ClO_4 and NH_4PF_6 lattices 214 (1997) 425
- Byrd, E.F.C., see Chesnut, D.B. 213 (1996) 153
- Camargo, A.C., J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés, An ab initio perturbed ion study of structural properties of TiO_2 , SnO_2 and GeO_2 rutile lattices 212 (1996) 381
- Campagne, B., see Brunel, M. 218 (1997) 301
- Cannistraro, S., see Lamanna, R. 213 (1996) 95
- Cannistraro, S., see Rocchi, C. 214 (1997) 261
- Canty, J.F., E.G. Stone, S.B.H. Bach and D.W. Ball, Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations 216 (1997) 81
- Canva, M., see Brunel, M. 218 (1997) 301
- Cao, H., see Xie, X. 213 (1996) 133
- Cao, X., H. Liu and N. Chen, Classification of Cm I energy levels using PCA-BPN and PCA-NLM 220 (1997) 289

- Cao, Z.L., see Yu, X.P. 215 (1997) 1
- Capobianco, J.A., P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli, Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er^{3+} in YVO_4 214 (1997) 329
- Carbognani, A., see Ferrari, L. 215 (1997) 37
- Carrington Jr., T., see Krishnan, M.S. 219 (1997) 31
- Caspary, N., B.E. Wurfel, A.M. Smith and V.E. Bondybey, Nonradiative processes and infrared emission in matrix isolated ND 220 (1997) 241
- Cassidei, L., see Petrella, G. 216 (1997) 391
- Castellano, E., see Croce, A.E. 211 (1996) 215
- Cattaneo, P. and M. Persico, Ab initio determination of quasi-diabatic states for multiple reaction pathways 214 (1997) 49
- Cavalli, E., see Capobianco, J.A. 214 (1997) 329
- Cavalli, S., see Aquilanti, V. 214 (1997) 1
- Cerny, D., R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota, Analysis of the $D'2_g-A'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry 216 (1997) 207
- Cerny, U., see Obrebski, A. 212 (1996) 311
- Chaillet, M., see Habas, M.-P. 219 (1997) 63
- Chakravorty, S.J., see Zheng, Y. 212 (1996) 269
- Chakravorty, S.J., see Rolke, J. 215 (1997) 191
- Champagne, B., see Jacquemin, D. 213 (1996) 217
- Chan, W.F., see Olney, T.N. 218 (1997) 127
- Chandra, A.K., see Sreedhara Rao, V. 214 (1997) 103
- Chang, C.H., see Hayashi, M. 217 (1997) 259
- Chang, I., H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak, Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy 212 (1996) 221
- Chapo, C., see Szczepanski, J. 211 (1996) 359
- Chapuisat, X., C. Saint-Espès, C. Zuhrt and L. Zülicke, A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH 217 (1997) 43
- Chaput, F., see Kulikov, S.G. 216 (1997) 147
- Chaput, F., see Brunel, M. 218 (1997) 301
- Chaquin, P., see Bahou, M. 216 (1997) 105
- Chassé, T., see Franke, R. 220 (1997) 299
- Chauvet, J.-P., see Laguitton-Pasquier, H. 212 (1996) 437
- Che, J., see Yan, Y.J. 217 (1997) 297
- Chen, I.-C., see Lee, S.-H. 220 (1997) 175
- Chen, N., see Cao, X. 220 (1997) 289
- Chen, Z., see Shapiro, M. 217 (1997) 325
- Chesnut, D.B. and E.F.C. Byrd, The use of locally dense basis sets in correlated NMR chemical shielding calculations 213 (1996) 153
- Chesnut, D.B., On the calculation of hydrogen NMR chemical shielding 214 (1997) 73
- Chikhaoui, A. and E.V. Kustova, Effect of strong excitation of the CO_2 asymmetric mode on transport properties 216 (1997) 297
- Chong, D.P., see Pulfer, M. 216 (1997) 91
- Chong, D.P., see Hu, C.-H. 216 (1997) 99
- Chowdhury, P.K., see Schmid, R.P. 218 (1997) 291
- Christen, C., see Dietz, F. 218 (1997) 43

- Chu, S.-I., see Tong, X.-M. 217 (1997) 119
- Chua, M. and P.A. Tanner, Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $\text{Cs}_2\text{NaCeCl}_6$ 218 (1997) 83
- Churassy, S., see Cerny, D. 216 (1997) 207
- Ciriaco, F., see Petrella, G. 216 (1997) 391
- Clark, B.K., J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming, Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit 213 (1996) 229
- Clark, N.A., see Ginzburg, V.V. 214 (1997) 253
- Clark, R.J.H., see Svendsen, C. 215 (1997) 89
- Clark, R.J.H., see Torii, H. 216 (1997) 67
- Clogston, A.M., see McDowell, H.K. 211 (1996) 91
- Cobos, C.J., see Croce, A.E. 211 (1996) 215
- Coletti, C., see Aquilanti, V. 214 (1997) 1
- Collet, A., see Laguitton-Pasquier, H. 212 (1996) 437
- Colomban, P., see Fillaux, F. 216 (1997) 281
- Comes, F.J., see Lock, M. 213 (1996) 385
- Compostizo, A., C. Martín, R.G. Rubio and A. Crespo Colin, Temperature dependence of the density of an ionic micellar system near the critical point 212 (1996) 301
- Consolati, G. and F. Quasso, Positronium dynamics in aqueous solutions of ionic surfactants 213 (1996) 449
- Contador, J.C., M.A. Aguilar and F.J.O. del Valle, Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium-water clusters 214 (1997) 113
- Cooksy, A.L., see Wang, H. 213 (1996) 139
- Cooper, D.L., see Gianturco, F.A. 215 (1997) 227
- Cooper, D.R., see Yench, A.J. 216 (1997) 227
- Cooper, G., see Au, J.W. 215 (1997) 397
- Cooper, G., see Olney, T.N. 218 (1997) 127
- Cooper, J.L., see Ahmed, M. 219 (1997) 333
- Coriani, S., A. Rizzo, K. Ruud and T. Helgaker, Cotton-Mouton effect and shielding polarizabilities of ethylene: an MCSCF study 216 (1997) 53
- Cormack, A.J., A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King, High-resolution threshold photoelectron spectroscopy of molecular fluorine 213 (1996) 439
- Cormack, A.J., see Yench, A.J. 216 (1997) 227
- Coropceanu, V.P., F.G. Paladi, S.I. Boldyrev and V.J. Gamurar, Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties 219 (1997) 1
- Cortés, J. and E. Valencia, Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy 219 (1997) 235
- Coussan, S., Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine, Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations 219 (1997) 221
- Cowdery-Corvan, J.R., see Sinicropi, J.A. 218 (1997) 331
- Crespo Colin, A., see Compostizo, A. 212 (1996) 301
- Croce, A.E., C.J. Cobos and E. Castellano, Experimental and theoretical study of the recombination reaction of FC(O)O radicals 211 (1996) 215
- Croci, M., see Güttler, F. 211 (1996) 421
- Cuadros, F., A. Mulero and W. Okrasinski, Thermodynamic shift from three- to two-dimensional systems 218 (1997) 235

- Cukier, R.I., see Morillo, M. 212 (1996) 157
- Cukier, R.I., C. Denk and M. Morillo, Control of tunneling processes with an external field in a four-level system: an analytic approach 217 (1997) 179
- Czerwiński, M. and J. Dąbrowski, Spin–spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster 213 (1996) 45
- Czerwiński, M. and J. Dąbrowski, Spin–spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster (Chem. Phys. 213 (1996) 45–62) 216 (1997) 295
- Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Calculation of ground- and excited-state potential energy curves for the Hg_2 molecule in a pseudopotential approach 214 (1997) 277
- Dąbrowski, J., see Czerwiński, M. 213 (1996) 45
- Dąbrowski, J., see Czerwiński, M. 216 (1997) 295
- Da Graça Miguel, M., see Ferreira Marques, M.F. 220 (1997) 233
- Dähne, L., see Werncke, W. 216 (1997) 337
- Dapprich, J., see Widengren, J. 216 (1997) 417
- Dargelos, A., see Pericou-Cayere, M. 214 (1997) 81
- Das, P.K., see Ray, P.C. 211 (1996) 499
- Dashevskaya, E.I., see Rosenblum, I. 213 (1996) 243
- Da Silva, A.B.F., see Jorge, F.E. 216 (1997) 317
- Davidson, E.R., see Zheng, Y. 212 (1996) 269
- Davidson, E.R., see Rolke, J. 215 (1997) 191
- De Castro, E.V.R., see Jorge, F.E. 216 (1997) 317
- Decleva, P., see Fronzoni, G. 220 (1997) 15
- Dedonder-Lardeux, C., C. Jouvet, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard, Intracuster ion–molecule reactions induced by the synchrotron radiation in allyl bromide–ammonia clusters 212 (1996) 371
- De Haas, M.P., see Warman, J.M. 212 (1996) 183
- De Lara-Castells, M.P., see Gianturco, F.A. 219 (1997) 117
- Delcourt, O., M. Descamps, J. Even, M. Bertault and J.F. Willart, Peculiarities of the enthalpy relaxation of a glassy crystal 215 (1997) 51
- Delgado-Barrio, G., see Buonomo, E. 218 (1997) 71
- De Lima, A.P., see Ferreira Marques, M.F. 220 (1997) 233
- Délugeard, Y., see Even, J. 213 (1996) 357
- Del Valle, F.J.O., see Contador, J.C. 214 (1997) 113
- Delysse, S., P. Raimond and J.-M. Nunzi, Two-photon absorption in non-centrosymmetric dyes 219 (1997) 341
- Deng, C.-H., see Wang, Y.-X. 214 (1997) 33
- Denk, C., see Morillo, M. 212 (1996) 157
- Denk, C., see Cukier, R.I. 217 (1997) 179
- De Oliveira, L.F.C., see Ribeiro, M.C.C. 217 (1997) 71
- Descamps, M., see Delcourt, O. 215 (1997) 51
- DeWitt, M.J., D.W. Peters and R.J. Levis, Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation 218 (1997) 211
- Dexpert-Ghys, J., see Tanner, P.A. 215 (1997) 125
- Dickinson, A.S., see Viehland, L.A. 211 (1996) 1
- Dietter, J. and H. Morgner, Structure and dynamics at the surface of a concentrated aqueous solution of CsF 220 (1997) 261
- Dietz, F., N. Tyutyulkov, C. Christen and K. Lüders, Nature of the magnetic interaction of Wurster's radicals in the solid state 218 (1997) 43

- Dietz, H., A. Materny and V. Engel, Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule 217 (1997) 249
- Dimicoli, I., see Dedonder-Lardeux, C. 212 (1996) 371
- Ding, S., see Guan, D. 218 (1997) 1
- Dobrin, S., P. Kaszynski, S. Ikeda and J. Waluk, Photophysics of *trans*-stilbene analogues: indolo[3,2-*b*]indole and its heterosubstituted sulfur and selenium derivatives 216 (1997) 179
- Domcke, W., see Wolfseder, B. 217 (1997) 275
- Donaldson, D.J., see Randall, K.L. 211 (1996) 377
- Donovan, R.J., see Cormack, A.J. 213 (1996) 439
- Dore, J.C., see Bakó, I. 216 (1997) 119
- Dreizler, H., see Alonso, J.L. 218 (1997) 267
- Drese, K. and M. Holthaus, Ultracold atoms in modulated standing light waves 217 (1997) 201
- Drobizhev, M.A., M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky, Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye 211 (1996) 455
- Duang, W., see Xie, X. 213 (1996) 133
- Dugourd, Ph., D. Rayane, R. Antoine and M. Broyer, Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process 218 (1997) 163
- Dunne, L.J., see Lukhezo, M. 220 (1997) 53
- Duplâtre, G., see Ferreira Marques, M.F. 220 (1997) 233
- Duran, M., see Luis, J.M. 217 (1997) 29
- Durig, J.R., S. Shen, W. Zhao and L. Zhou, Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions 213 (1996) 165
- Durig, J.R., Y. Li and Y. Jin, Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra 213 (1996) 181
- Dyke, J.M., see Mack, P. 218 (1997) 243
- Dyre, J.C. and J.M. Jacobsen, Universality of anomalous diffusion in extremely disordered systems 212 (1996) 61
- Ebenhoch, J., see Bensasson, R.V. 215 (1997) 111
- Ebner, C., see Limtrakul, J. 215 (1997) 77
- Effenberger, F., see Steybe, F. 219 (1997) 317
- Eid, O.I., see Salih, N.A. 212 (1996) 409
- Eilmes, A., R.W. Munn, B. Pac and P. Petelenz, Charge-transfer states and the band gap in crystalline fullerene 214 (1997) 341
- Eisenhardt, C.G., S. Ring, H.-W. Jochims and H. Baumgärtel, Clusters containing BF₃, O(CH₃)₂ and aromatic compounds: An electron impact and photoionization study 216 (1997) 427
- Ekern, S., see Szczepanski, J. 211 (1996) 359
- Eland, J.H.D., P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson, Vibrational structure of the BrCN⁺ ion from high resolution photoelectron spectroscopy 212 (1996) 457
- Ellinger, Y., see Parisel, O. 212 (1996) 331
- Engdahl, A. and B. Nelander, IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes 213 (1996) 333
- Engdahl, A., see Kölm, J. 214 (1997) 313
- Engel, V., see Dietz, H. 217 (1997) 249
- Engkvist, O. and G. Karlström, A method to calculate the probability distribution for systems with large energy barriers 213 (1996) 63

- Enkvist, C., S. Lunell and S. Svensson, Experimental and theoretical study of the C_{1s} shakeup spectra from biphenyl and p-terphenyl 214 (1997) 123
- Eremenko, V.V., V.A. Karachevtsev and V.V. Slavin, Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA 216 (1997) 1
- Ermeneux, F.S., see Capobianco, J.A. 214 (1997) 329
- Eschrich, I., see Ruth, C. 213 (1996) 454
- Esmond, J.R., see Yoshino, K. 211 (1996) 387
- Esmond, J.R., see Yoshino, K. 215 (1997) 429
- Esser, B., see Ankerhold, U. 220 (1997) 393
- Evangelisti, S., see Bendazzoli, G.L. 215 (1997) 217
- Evangelisti, S., Carbon–oxygen clusters as hypothetical high energy-density materials 218 (1997) 21
- Even, J., M. Bertault, A. Girard and Y. Délugeard, Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP 213 (1996) 357
- Even, J., see Delcourt, O. 215 (1997) 51
- Fahr, A., P. Hassanzadeh, B. Laszlo and R.E. Huie, Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region 215 (1997) 59
- Fainberg, B.D. and B. Zolotov, Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing 216 (1997) 7
- Faure, J., see Laguitton-Pasquier, H. 212 (1996) 437
- Felfli, Z., I. Fomunung, D. Bessis and A.Z. Msezane, Generalized oscillator strengths for SF_6 in the S 2p inner-shell region 211 (1996) 325
- Fernández Gómez, M., see Kearley, G.J. 216 (1997) 323
- Ferrari, L. and A. Carbognani, Drift velocity of ions in lighter gases in electric and magnetic fields 215 (1997) 37
- Ferreira Marques, M.F., H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre, Effects of CCl_4 on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions 220 (1997) 233
- Fillaux, F., N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colombar, A. Gruger, A. Régis and L.T. Yu, Inelastic neutron scattering studies of polyanilines and partially deuterated analogues 216 (1997) 281
- Fischer, S.F., see Scharnagl, C. 212 (1996) 231
- Fischer, S.F., see Berlin, Y.A. 220 (1997) 25
- Fišer, J., see Vojtík, J. 218 (1997) 13
- Flad, H.-J., see Leininger, T. 217 (1997) 19
- Fleming, J.R., see Clark, B.K. 213 (1996) 229
- Fleurov, V., see Barkai, E. 212 (1996) 69
- Fominykh, N.G., see Franke, R. 216 (1997) 243
- Fomunung, I., see Felfli, Z. 211 (1996) 325
- Forney, D., see Freivogel, P. 216 (1997) 401
- Francisco, J.S., A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the $FCO + H_2 \rightarrow HFCO + H$ abstraction reaction 214 (1997) 213
- Francisco, J.S., see Aloisio, S. 219 (1997) 201
- Franke, R., S. Bender, J. Hormes, A.A. Pavlychev and N.G. Fominykh, A quasi-atomic treatment of chemical and structural effects on K-shell excitations in hexagonal and cubic BN crystals 216 (1997) 243

- Franke, R., T. Chassé, J. Reinhold, P. Streubel and R. Szargan, Extended Fenske-Hall LCAO MO calculations of core-level shifts in solid P compounds 220 (1997) 299
- Frantsuzov, P.A., see Burshtein, A.I. 212 (1996) 137
- Freivogel, P., M. Grutter, D. Forney and J.P. Maier, Infrared bands of mass-selected carbon chains C_n ($n = 8-12$) and C_n^- ($n = 5-10, 12$) in neon matrices 216 (1997) 401
- Frick, B., see Büttner, H.G. 214 (1997) 425
- Fronzoni, G. and P. Decleva, Highly correlated QDPT-CI calculations of valence and core photoelectron spectra of Ne 220 (1997) 15
- Fujimura, Y., see Watanabe, Y. 217 (1997) 317
- Galasso, V., Theoretical study of the low-lying excited states of ABCO, DABCO and homologous cage amines 215 (1997) 183
- Galaup, J.P., see Kulikov, S.G. 216 (1997) 147
- Galaup, J.P., see Arabei, S.M. 216 (1997) 163
- Gamurar, V.J., see Coropceanu, V.P. 219 (1997) 1
- Garay Salazar, M., J.M. Orea and A. González Ureña, On the determination of $D_0^0(\text{CaBr})$ from translational energy threshold measurements 216 (1997) 365
- Garnier, F., see Klein, G. 215 (1997) 131
- Gelinck, G.H., see Warman, J.M. 212 (1996) 183
- Gelize, M., see Pericou-Cayere, M. 214 (1997) 81
- Georges, R., see Mellouki, A. 220 (1997) 311
- Gericke, K.-H., see Lock, M. 213 (1996) 385
- Germain, A. and P. Millié, Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules 219 (1997) 265
- German, E.D., see Mertz, E.L. 215 (1997) 355
- Gerratt, J., see Gianturco, F.A. 215 (1997) 227
- Gerst, M., see Bensasson, R.V. 215 (1997) 111
- Ghosh, S.K., see Samanta, A. 214 (1997) 61
- Gianturco, F.A., S. Kumar and F. Schneider, Correlated electronic potential-energy surfaces for proton interactions with N_2 211 (1996) 33
- Gianturco, F.A., S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper, Interaction forces and energy transfer dynamics of $\text{LiH} (^1\Sigma^+)$ and helium atoms. I. The ab initio evaluation of the lowest potential energy surface 215 (1997) 227
- Gianturco, F.A., S. Kumar, S.K. Pathak, M. Raimondi and M. Sironi, Interaction forces and energy transfer dynamics of $\text{LiH} (^1\Sigma^+)$ and helium atoms. II. Rotationally inelastic collisions and excitation efficiency 215 (1997) 239
- Gianturco, F.A., see Buonomo, E. 218 (1997) 71
- Gianturco, F.A. and M.P. de Lara-Castells, Structure and anisotropy of ionic argon clusters using density functional models [Chem. Phys. 208 (1996) 25-34]. Erratum 219 (1997) 117
- Gingell, J.M., N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel, VUV optical-absorption and electron-energy-loss spectroscopy of formamide 220 (1997) 191
- Ginzburg, V.V., M.A. Glaser and N.A. Clark, A new potential for the description of intermolecular interactions for rigid biaxial molecules 214 (1997) 253
- Girard, A., see Even, J. 213 (1996) 357
- Gislason, E.A., see Song, J.-B. 212 (1996) 259
- Gislason, E.A., see Song, J.-B. 214 (1997) 23
- Glania, C., see Steybe, F. 219 (1997) 317
- Glasbeek, M., see Middelhoek, E.R. 211 (1996) 489

- Glaser, M.A., see Ginzburg, V.V. 214 (1997) 253
- Gliński, J., see Baranowski, A. 214 (1997) 143
- Gomez Llorente, J.M., see Zanardi, E.M. 217 (1997) 221
- González Ureña, A., see Garay Salazar, M. 216 (1997) 365
- González Ureña, A., see Orea, J.M. 220 (1997) 337
- Gorbach, V.V., see Petrov, E.G. 220 (1997) 249
- Gorbunov, A.V., see Kveder, V.V. 216 (1997) 407
- Gordillo, M.C. and C.P. Herrero, Al,Si ordering in chabazites: A Monte Carlo study 211 (1996) 81
- Gorin, T., H.J. Korsch and B. Mirbach, Phase-space localization and level spacing distributions for a driven rotor with mixed regular/chaotic dynamics 217 (1997) 145
- Goto, T., see Oeda, Y. 213 (1996) 421
- Götze, W. and L. Sjögren, Comments on the mode coupling theory for structural relaxation 212 (1996) 47
- Grahn, W., see Werncke, W. 216 (1997) 337
- Granucci, G., see Romstad, D. 219 (1997) 21
- Grebenshchikov, S.Yu., see Benderskii, V.A. 219 (1997) 119
- Green, N.J.B., R.D. Spencer-Smith and A.G. Rickerby, Recovering boundaries for partly diffusion-controlled reaction kinetics 212 (1996) 99
- Grifoni, M., L. Hartmann and P. Hänggi, Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations 217 (1997) 167
- Grigorenko, B.L., A.V. Nemukhin and V.A. Apkarian, Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He-Cl₂ and Ar-Cl₂ 219 (1997) 161
- Grisogono, A.M., see Zheng, Y. 212 (1996) 269
- Gross, A. and G.D. Billing, Isotope effects on the rate constants for the processes O₂ + O → O + O₂ and O₂ + O + Ar → O₃ + Ar. On a modified ground-state potential energy surface for ozone 217 (1997) 1
- Gruger, A., see Fillaux, F. 216 (1997) 281
- Gründel, M., see Ruth, C. 213 (1996) 454
- Grutter, M., see Freivogel, P. 216 (1997) 401
- Grycuk, T., see Roston, G.D. 213 (1996) 365
- Guan, D., X. Yi, S. Ding and B. Yang, Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface 218 (1997) 1
- Gudowska-Nowak, E., Dynamic effects in non-adiabatic charge transfer 212 (1996) 115
- Gudowska-Nowak, E., G. Papp and J. Brickmann, Two-level system with noise: Blue's function approach 220 (1997) 125
- Guest, M.F., see Palmer, M.H. 214 (1997) 191
- Güttler, F., M. Croci, A. Renn and U.P. Wild, Single molecule polarization spectroscopy: pentacene in p-terphenyl 211 (1996) 421
- Haarer, D., see Zilker, S.J. 220 (1997) 167
- Habas, M.-P., I. Baraille, C. Larrieu and M. Chaillet, Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine 219 (1997) 63
- Habdas, P., see Paluch, M. 213 (1996) 483
- Hall, G.E., see North, S.W. 211 (1996) 515
- Hamada, T., Rydberg basis set effects on ab initio second hyperpolarizabilities of H₂, C₆H₆ and CS₂ molecules 211 (1996) 171
- Han, R.S., see Yu, X.P. 215 (1997) 1

- Hands, I.D., see Andrews, D.L. 213 (1996) 277
- Handschuh, M., see Lorenz, W. 215 (1997) 139
- Handschuh, M., see Bergmann, F. 215 (1997) 157
- Hänggi, P., see Grifoni, M. 217 (1997) 167
- Hannongbua, S., see Tongraar, A. 219 (1997) 279
- Hanson, G.R., see Wilson, C.R. 217 (1997) 63
- Hanus, M., see Parisel, O. 212 (1996) 331
- Harryvan, D.H., see Muller, J.M. 211 (1996) 413
- Hartmann, H., see Chang, I. 212 (1996) 221
- Hartmann, L., see Grifoni, M. 217 (1997) 167
- Hase, W.L., see Wang, H. 212 (1996) 247
- Hassanzadeh, P., see Fahr, A. 215 (1997) 59
- Hawlicka, E. and D. Swiatla-Wojcik, Molecular dynamics simulation of NaCl solutions in methanol-water mixtures. Intramolecular vibrations of the solvent components 218 (1997) 49
- Hayashi, H., see Salikhov, K.M. 220 (1997) 355
- Hayashi, M., T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer, Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases 217 (1997) 259
- Hayes, M.A., see Holland, D.M.P. 219 (1997) 91
- Heinecke, R., see Lossau, H. 213 (1996) 1
- Helgaker, T., see Coriani, S. 216 (1997) 53
- Helmi, M.S., see Roston, G.D. 213 (1996) 365
- Herman, M., see Mellouki, A. 220 (1997) 311
- Hernandez, J.M., see Martínez, H. 215 (1997) 285
- Herrero, C.P., see Gordillo, M.C. 211 (1996) 81
- Hikida, T., see Matsushita, Y. 213 (1996) 413
- Hill, T.J., see Bensasson, R.V. 215 (1997) 111
- Hirao, K., see Tajima, N. 218 (1997) 257
- Hiraya, A., see Kanda, K. 218 (1997) 199
- Hoffman, D.K., see Althorpe, S.C. 217 (1997) 289
- Holland, D.M.P., D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg, A photoabsorption, photodissociation and photoelectron spectroscopy study of C₂H₄ and C₂D₄ 219 (1997) 91
- Holmén, A., see Broo, A. 211 (1996) 147
- Holthaus, M., see Drese, K. 217 (1997) 201
- Honjou, N. and E. Miyoshi, Ab initio study on the electronic structure of the 4²Σ⁺ and 5²Σ⁺ excited states of CO⁺ 212 (1996) 363
- Hopkirk, A., see Cormack, A.J. 213 (1996) 439
- Hopkirk, A., see Ahmed, M. 219 (1997) 333
- Hörhold, H.-H., see Tak, Y.-H. 212 (1996) 471
- Hormes, J., see Franke, R. 216 (1997) 243
- Hornos, J.E.M., see Bernardes, E.S. 213 (1996) 17
- Hornos, Y.M.M., see Bernardes, E.S. 213 (1996) 17
- Horowitz, G., see Klein, G. 215 (1997) 131
- Hottmann, K., see Loch, R. 220 (1997) 207
- Hottmann, K., see Loch, R. 220 (1997) 217
- Hu, C.-H., see Pulfer, M. 216 (1997) 91

- Hu, C.-H. and D.P. Chong, Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules 216 (1997) 99
- Hu, Y., W. Lu and S. Yang, Intermolecular vibrations of the van der Waals complex $p\text{-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$ 218 (1997) 325
- Huber, H., see Welker, M. 213 (1996) 253
- Hubinger, S., see Nee, J.B. 211 (1996) 403
- Hughes, C., see Ahmed, M. 219 (1997) 333
- Hughes, J.M. and E.I. von Nagy-Felsobuki, Ab initio calculations of the rovibrational states of He_2N^{2+} 211 (1996) 135
- Huie, R.E., see Fahr, A. 215 (1997) 59
- Hulsman, H., Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion 217 (1997) 107
- Hunter, G., see Kudryavtsev, A.B. 215 (1997) 419
- Huxley, D.W., see Bakó, I. 216 (1997) 119
- Igarashi, S., see Nonomura, Y. 220 (1997) 155
- Igualada, J.A., see Camargo, A.C. 212 (1996) 381
- Ikeda, S., see Dobrin, S. 216 (1997) 179
- Il'ichev, Yu.V., W. Kühnle and K.A. Zachariasse, Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans-cis photoisomerisation 211 (1996) 441
- Inard, D., see Cerny, D. 216 (1997) 207
- Inoue, H., see Nonomura, Y. 220 (1997) 155
- Ito, F., see Schmid, R.P. 218 (1997) 291
- Ito, K., see Yoshino, K. 211 (1996) 387
- Ito, K., see Yoshino, K. 215 (1997) 429
- Ivanov, V.S. and V.B. Sovkov, An IPA procedure for bound-continuum diatomic transition intensities 213 (1996) 295
- Iwata, S., see Li, Y. 219 (1997) 209
- Jäckel, J.-G., R. Schmid, H. Jones, T. Nakanaga and H. Takeo, The van der Waals vibrational frequencies of the aniline-carbon monoxide complex in its S_1 state 215 (1997) 291
- Jacobsen, J.M., see Dyre, J.C. 212 (1996) 61
- Jacquemin, D., B. Champagne, J.-M. André and B. Kirtman, Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains 213 (1996) 217
- Jacques, P., see Allonas, X. 215 (1997) 371
- Jäger, F., see Ujj, L. 212 (1996) 421
- Jäger, F., see Ujj, L. 217 (1997) 115
- Jakubetz, W. and B.L. Lan, A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces 217 (1997) 375
- Jas, G.S. and K. Kuczera, Ab initio calculations of S_1 excited state vibrational spectra of benzene, naphthalene and anthracene 214 (1997) 229
- Jerie, K., see Baranowski, A. 214 (1997) 143
- Jiang, K., see Zheng, H. 211 (1996) 507
- Jin, Y., see Durig, J.R. 213 (1996) 181
- Jochims, H.W., see Biehl, H. 214 (1997) 367

- Jochims, H.-W., see Eisenhardt, C.G. 216 (1997) 427
- Johannes, H.-H., see Werncke, W. 216 (1997) 337
- Johnson, M.R., M. Neumann, B. Nicolai, P. Smith and G.J. Kearley, The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid 215 (1997) 343
- Johr, T., see Werncke, W. 216 (1997) 337
- Jones, A.L., A.J. Blake, L. Torop and D.G. McCoy, An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region 211 (1996) 291
- Jones, H., see Jäckel, J.-G. 215 (1997) 291
- Jones, H., see Schmid, R.P. 218 (1997) 291
- Jones, N.C., see O'Connor, C.S.S. 214 (1997) 131
- Jonsson, T., see Lossau, H. 213 (1996) 1
- Jonusauskas, G., see Abraham, E. 214 (1997) 409
- Jonusauskas, G., see Abraham, E. 219 (1997) 73
- Jorge, F.E., E.V.R. de Castro and A.B.F. da Silva, Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree-Fock method 216 (1997) 317
- Jørgensen, J.S., J.B. Pedersen and A.I. Shushin, Magnetic field dependent yield of geminate radical pair recombination in micelles. Effect of intraradical spin lattice relaxation 211 (1996) 235
- Jouvet, C., see Dedonder-Lardeux, C. 212 (1996) 371
- Jovanovic-Kurepa, J., D.D. Markusev and M. Terzic, Multiple absorption and relaxation processes in SF₆-CH₄ mixtures: an experimental study 211 (1996) 347
- Jundt, C., see Klein, G. 215 (1997) 131
- Jursic, B.S., Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl 219 (1997) 57
- Kabro, P., see Capobianco, J.A. 214 (1997) 329
- Kalotas, T.M., see Mellor, W.E. 219 (1997) 257
- Kanda, K., S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake, Photodissociation spectroscopy of ICN in the vacuum ultraviolet region 218 (1997) 199
- Kaps, T., see Obrebski, A. 212 (1996) 311
- Karachevtsev, V.A., see Eremenko, V.V. 216 (1997) 1
- Karafiloglou, P., Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state 214 (1997) 171
- Karlsson, L., see Eland, J.H.D. 212 (1996) 457
- Karlsson, L., see Holland, D.M.P. 219 (1997) 91
- Karlström, G., see Engkvist, O. 213 (1996) 63
- Kaszynski, P., see Dobrin, S. 216 (1997) 179
- Katsumata, S., see Kanda, K. 218 (1997) 199
- Kausche, T., see Richter, A. 214 (1997) 321
- Kearley, G.J., see Büttner, H.G. 214 (1997) 425
- Kearley, G.J., see Neumann, M. 215 (1997) 253
- Kearley, G.J., see Johnson, M.R. 215 (1997) 343
- Kearley, G.J., J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez, Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine 216 (1997) 323

- Keith, T.A., Calculation of magnetizabilities using GIAO current density distributions 213 (1996) 123
- Kerdcharoen, T., K.R. Liedl and B.M. Rode, A QM/MM simulation method applied to the solution of Li^+ in liquid ammonia 211 (1996) 313
- Khasanov, S.S., see Kveder, V.V. 216 (1997) 407
- Khmelninskii, I.V., see Makarov, V.I. 214 (1997) 151
- Kim, K.-R., see Lee, D.J. 214 (1997) 183
- King, G.C., see Cormack, A.J. 213 (1996) 439
- King, G.C., see Yench, A.J. 216 (1997) 227
- Kirtman, B., see Jacquemin, D. 213 (1996) 217
- Klafter, J., see Zumofen, G. 212 (1996) 89
- Kleima, F.J., see Visser, H.M. 215 (1997) 299
- Klein, G., C. Jundt, B. Sipp, A.A. Villaeys, A. Boeglin, A. Yassar, G. Horowitz and F. Garnier, Femtosecond dynamics of excited states in sexithiophene thin films 215 (1997) 131
- Knast, K., Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules 213 (1996) 465
- Knüpling, M., J.T. Törring and S. Un, The relationship between the molecular structure of semiquinone radicals and their g -values 219 (1997) 291
- Kohlmeyer, A., W. Witschel and E. Spohr, Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model 213 (1996) 211
- Kölm, J., A. Engdahl, O. Schrems and B. Nelander, A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices 214 (1997) 313
- Kolodziejski, M., G. Waliszewska and H. Abramczyk, Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms 213 (1996) 341
- Kompa, C., see Lossau, H. 213 (1996) 1
- Konarev, D.V., see Kveder, V.V. 216 (1997) 407
- Kondow, T., see Kanda, K. 218 (1997) 199
- Kono, H., see Watanabe, Y. 217 (1997) 317
- Koper, M.T.M. and W. Schmickler, A Kramers reaction rate theory for electrochemical ion transfer reactions 211 (1996) 123
- Koper, M.T.M., J.-H. Mohr and W. Schmickler, Quantum effects in adiabatic electrochemical electron-transfer reactions 220 (1997) 95
- Koperski, J., Potential energy curve of the $\text{XO}^+(\text{}^1\Sigma^+)$ ground state of HgAr determined from $\text{A0}^+(\text{}^3\Pi) \rightarrow \text{XO}^+$ and $\text{B1}(\text{}^3\Sigma^+) \rightarrow \text{XO}^+$ fluorescence spectra 211 (1996) 191
- Koperski, J., Potential energy curve of the $\text{XO}^+(\text{}^1\Sigma^+)$ ground state of HgAr determined from $\text{A0}^+(\text{}^3\Pi) \rightarrow \text{XO}^+$ and $\text{B1}(\text{}^3\Sigma^+) \rightarrow \text{XO}^+$ fluorescence spectra (Chemical Physics 211 (1996) 191-201) 214 (1997) 431
- Korolkov, M.V., J. Manz and G.K. Paramonov, Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association 217 (1997) 341
- Korsch, H.J., see Gorin, T. 217 (1997) 145
- Kosterev, A.A., A.A. Makarov, A.L. Malinovsky and E.A. Ryabov, Fast collision-induced redistribution of vibrational energy in halogenated methanes 219 (1997) 305
- Kouri, D.J., see Althorpe, S.C. 217 (1997) 289
- Kouznetsova, T.V., see Kudryavtsev, A.B. 215 (1997) 419
- Kraemer, W.P., see Sauer, S.P.A. 214 (1997) 91
- Krämer, P., see Steybe, F. 219 (1997) 317
- Krause, J.L., see Yan, Y.J. 217 (1997) 297

- Krishnan, M.S. and T. Carrington Jr., Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms 219 (1997) 31
- Kristyan, S., see Boughton, J.W. 214 (1997) 219
- Krupyanskii, Yu., see Chang, I. 212 (1996) 221
- Kuczera, K., see Jas, G.S. 214 (1997) 229
- Kudryavtsev, A.B., T.V. Kouznetsova, W. Linert and G. Hunter, A study of the hydration of aluminate minerals based on the measurements of the mean and the variance of the proton magnetic resonance relaxation rate 215 (1997) 419
- Kühnle, W., see Il'ichev, Yu.V. 211 (1996) 441
- Kuřak, L., see Bojarski, P. 220 (1997) 323
- Kulikov, S.G., A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot, Sol-gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion 216 (1997) 147
- Kulikov, S.G., see Arabei, S.M. 216 (1997) 163
- Kumada, T., Y. Aratono and T. Miyazaki, Time evolution of the rate constant for the tunneling reaction $H_2 + D \rightarrow H + HD$ in solid D_2-H_2 mixtures at very low temperature 212 (1996) 177
- Kumar, S., see Gianturco, F.A. 211 (1996) 33
- Kumar, S., see Gianturco, F.A. 215 (1997) 227
- Kumar, S., see Gianturco, F.A. 215 (1997) 239
- Kummer, A., see Lossau, H. 213 (1996) 1
- Küster, J., see Schael, F. 218 (1997) 175
- Kustova, E.V., see Chikhaoui, A. 216 (1997) 297
- Kuznetsov, A.M., see Mertz, E.L. 215 (1997) 355
- Kuznetsov, An.M. and W. Lorenz, Electronic charge density transfer along a constrained reaction path from a hydronium ion configuration into a hydrogen chemisorption state on Cu(100) 214 (1997) 243
- Kveder, V.V., E.A. Steinman, B.Zh. Narymbetov, S.S. Khasanov, L.P. Rozenberg, R.P. Shibaeva, A.V. Bazhenov, A.V. Gorbunov, M.Yu. Maksimuk, D.V. Konarev, R.N. Lyubovskaya and Yu.A. Ossipyan, Crystal structure and photoluminescence of single crystals of fullerene-9,9'-trans-bis(telluraxanthenyl) molecular complex: $C_{26}H_{18}Te_2 \cdot C_{60} \cdot CS_2$ 216 (1997) 407
- Laguitton-Pasquier, H., R. Pansu, J.-P. Chauvet, A. Collet, J. Faure and R. Lapouyade, The charge transfer state of excited bianthryl and a derivative: solvatochromism, emission CT spectra broadening in homogeneous solvents 212 (1996) 437
- Lamanna, R. and S. Cannistraro, Effect of ethanol addition upon the structure and the cooperativity of the water H bond network 213 (1996) 95
- Lamrini, M., see Cerny, D. 216 (1997) 207
- Lan, B.L., see Jakubetz, W. 217 (1997) 375
- Land, E.J., see Bensasson, R.V. 215 (1997) 111
- Laplaza, A., see Orea, J.M. 220 (1997) 337
- Lapouyade, R., see Laguitton-Pasquier, H. 212 (1996) 437
- Lapouyade, R., see Abraham, E. 214 (1997) 409
- Lapouyade, R., see Abraham, E. 219 (1997) 73
- Larrieu, C., see Habas, M.-P. 219 (1997) 63
- Larzillière, M., see Boudjarane, K. 211 (1996) 393
- Laszlo, B., see Fahr, A. 215 (1997) 59

- Latajka, Z. and S. Scheiner, Structure, energetics and vibrational spectra of dimers, trimers, and tetramers of HX (X = Cl, Br, I) 216 (1997) 37
- Lau, A., see Werncke, W. 216 (1997) 337
- Lawley, K.P., see Cormack, A.J. 213 (1996) 439
- Leach, S., see Bensasson, R.V. 215 (1997) 111
- Lee, A.R., see Mellor, W.E. 219 (1997) 257
- Lee, D.J. and K.-R. Kim, On the degrees of circularity for various kinds of polarized light in a nonpolar liquid mixture 214 (1997) 183
- Lee, S.-H. and I.-C. Chen, Non-exponential decays of the S_1 vibronic levels of acetaldehyde 220 (1997) 175
- Lee, S.-L., see Slanina, Z. 219 (1997) 193
- Legay, F., see Legay-Sommaire, N. 211 (1996) 367
- Legay-Sommaire, N. and F. Legay, Isotope effects in the photochemical formation of HHgCH_3 and DHgCD_3 in nitrogen and methane matrices 211 (1996) 367
- Lehr, L., J. Manz and W.H. Miller, A classical approach to resonant low-energy electron scattering off molecules: application to the a_1 -shape resonance of CF_3Cl 214 (1997) 301
- Leininger, T., A. Berning, A. Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad, Spin-orbit interaction in heavy group 13 atoms and TlAr 217 (1997) 19
- Leroux, B., H. Bizot, J.W. Brady and V. Tran, Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose 216 (1997) 349
- Lesarri, A., see Alonso, J.L. 218 (1997) 267
- Levine, R.D., see Raz, T. 213 (1996) 263
- Levis, R.J., see DeWitt, M.J. 218 (1997) 211
- Leygue, N., see Fillaux, F. 216 (1997) 281
- Leyh, B., see Locht, R. 220 (1997) 207
- Leyh, B., see Locht, R. 220 (1997) 217
- Leytner, S., see Mellouki, A. 220 (1997) 311
- Li, M.-M., see Ong, P.P. 211 (1996) 115
- Li, Y., see Durig, J.R. 213 (1996) 181
- Li, Y. and S. Iwata, Theoretical study of cyclic radicals NO_x ($x = 2-6$) 219 (1997) 209
- Liedl, K.R., see Kerdcharoen, T. 211 (1996) 313
- Lifshitz, A. and H. Teitelbaum, The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions 219 (1997) 243
- Limtrakul, J., P. Treesukol, C. Ebner, R. Sansone and M. Probst, Structures and potential energy surface of Faujasitic zeolite/water 215 (1997) 77
- Lin, J., see Tanner, P.A. 215 (1997) 125
- Lin, M.C., see Boughton, J.W. 214 (1997) 219
- Lin, S.-H., see Mebel, A.M. 215 (1997) 329
- Lin, S.H., see Hayashi, M. 217 (1997) 259
- Linares, J., see Varret, F. 212 (1996) 487
- Lindgren, M., see Salih, N.A. 212 (1996) 409
- Linert, W., see Kudryavtsev, A.B. 215 (1997) 419
- Liu, H., see Cao, X. 220 (1997) 289
- Llusar, R., see Camargo, A.C. 212 (1996) 381
- Locht, R., B. Leyh, K. Hottmann and H. Baumgärtel, The photoabsorption spectrum of vinylchloride ($\text{C}_2\text{H}_3\text{Cl}$) in the 8–12 eV range 220 (1997) 207
- Locht, R., B. Leyh, K. Hottmann and H. Baumgärtel, The He(I) , threshold photoelectron and constant ion state spectroscopy of vinylchloride ($\text{C}_2\text{H}_3\text{Cl}$) 220 (1997) 217

- Lock, M., K.-H. Gericke and F.J. Comes, Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H(D)} + \text{N}_3$ 213 (1996) 385
- Logan, D., C.A. Wight and V.A. Apkarian, Vibron-mediated electronic relaxation in crystalline chlorine 217 (1997) 99
- Löhmansröben, H.-G., see Schael, F. 218 (1997) 175
- Longo, E., see Camargo, A.C. 212 (1996) 381
- Lopes Gil, C., see Ferreira Marques, M.F. 220 (1997) 233
- López, J.C., see Alonso, J.L. 218 (1997) 267
- López González, J.J., see Kearley, G.J. 216 (1997) 323
- Lorenz, W., see Kuznetsov, An.M. 214 (1997) 243
- Lorenz, W., M. Handschuh and F. Bergmann, Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation 215 (1997) 139
- Lorenz, W., see Bergmann, F. 215 (1997) 157
- Lorenzo, F.J., see Alonso, J.L. 218 (1997) 267
- Lossau, H., A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle, Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions 213 (1996) 1
- Loutellier, A., see Coussan, S. 219 (1997) 221
- Lu, W., see Hu, Y. 218 (1997) 325
- Lüders, K., see Dietz, F. 218 (1997) 43
- Luis, J.M., J. Martí, M. Duran and J.L. Andrés, Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation 217 (1997) 29
- Lukhezo, M., L.J. Dunne, B.G. Reuben and M.S. Verrall, Statistical mechanical treatment of reactive solvent extraction 220 (1997) 53
- Lukin, L.V., see Brazgun, F.F. 211 (1996) 469
- Lund, A., see Salih, N.A. 212 (1996) 409
- Lundqvist, M., see Eland, J.H.D. 212 (1996) 457
- Lunell, S., see Enkvist, C. 214 (1997) 123
- Lyubovskaya, R.N., see Kveder, V.V. 216 (1997) 407
- Mack, P., J.M. Dyke and T.G. Wright, Calculated thermodynamics of reactions involving $\text{NO}^+ \cdot \text{X}$ complexes (where $\text{X} = \text{H}_2\text{O}, \text{N}_2$ and CO_2) 218 (1997) 243
- MacKenzie, V.J., see Sinha, H.K. 213 (1996) 397
- Maclagan, R.G.A.R., see Viehland, L.A. 211 (1996) 1
- Maeda, K., see Tarasov, V.F. 212 (1996) 353
- Magin, E.H., see Sinicropi, J.A. 218 (1997) 331
- Maier, J.P., see Freivogel, P. 216 (1997) 401
- Makarov, A.A., see Kosterev, A.A. 219 (1997) 305
- Makarov, V.I. and I.V. Khmelinskii, Magnetic field effect of the fluorescence of gaseous NO_2 excited to the $^2\text{B}_2$ and $^2\text{B}_1$ states (Chemical Physics 207 (1996) 115-136) 214 (1997) 151
- Maksimuk, M.Yu., see Kveder, V.V. 216 (1997) 407
- Malinovsky, A.L., see Kosterev, A.A. 219 (1997) 305
- Manceron, L., see Tremblay, B. 218 (1997) 37
- Mansfield, M.W.D., see Ruth, A.A. 217 (1997) 83

- Manz, J., see Lehr, L. 214 (1997) 301
Manz, J., see Korolkov, M.V. 217 (1997) 341
Marković, N., T.D. Sewell, S. Nordholm and A. Miklavc, An improved classical approach quantum encounter treatment of collision-induced vibrational energy transfer. Application to He + CO ($n_i = 1, 2$) 211 (1996) 277
Marković, N., see Svanberg, M. 220 (1997) 137
Markusev, D.D., see Jovanovic-Kurepa, J. 211 (1996) 347
Maroulis, G. and C. Pouchan, Dipole polarizability and hyperpolarizability of FCN, ClCN, BrCN and ICN 215 (1997) 67
Martí, J., see Luis, J.M. 217 (1997) 29
Martín, C., see Compostizo, A. 212 (1996) 301
Martin, J.-P., see Porshnev, P.I. 213 (1996) 111
Martinez, H. and A. Amaya-Tapia, Translational spectroscopy of H^- produced by collision induced dissociation of H_3^+ on He 211 (1996) 299
Martínez, H. and J.M. Hernandez, Single electron capture in low-energy Kr^+ -He collisions 215 (1997) 285
Martrenchard-Barra, S., see Dedonder-Lardeux, C. 212 (1996) 371
Mason, N.J., see Gingell, J.M. 220 (1997) 191
Mata, S., see Alonso, J.L. 218 (1997) 267
Mataras, D., see Stamou, S. 218 (1997) 57
Materny, A., see Dietz, H. 217 (1997) 249
Matsui, A.H., see Oeda, Y. 213 (1996) 421
Matsui, T., see Yoshino, K. 211 (1996) 387
Matsui, T., see Yoshino, K. 215 (1997) 429
Matsushima, Y., see Oeda, Y. 213 (1996) 421
Matsushita, Y., Y. Yamaguchi and T. Hikida, The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase 213 (1996) 413
Matyushov, D.V., Solvent reorganization energy of electron transfer in weakly polar solvents 211 (1996) 47
Maus, M. and W. Rettig, The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds 218 (1997) 151
May, V., see Schirrmeister, D.H. 220 (1997) 1
May, V., see Petrov, E.G. 220 (1997) 249
McCarthy, I.E., see Rolke, J. 215 (1997) 191
McCoy, D.G., see Jones, A.L. 211 (1996) 291
McDowell, H.K. and A.M. Clogston, Maximum entropy imaging and quantum molecular timescale generalized Langevin equation theory 211 (1996) 91
McGarvey, D.J., see Bensasson, R.V. 215 (1997) 111
McNab, H., see Palmer, M.H. 214 (1997) 191
Mebel, A.M. and S.-H. Lin, Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra 215 (1997) 329
Mebel, A., see Hayashi, M. 217 (1997) 259
Mellor, W.E., A.R. Lee and T.M. Kalotas, Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials 219 (1997) 257
Mellouki, A., R. Georges, M. Herman, D.L. Snavely and S. Leytner, Spectroscopic investigation of ground state pyrrole ($^{12}C_4H_5N$): the N-H stretch 220 (1997) 311
Meredith, A.W., L. Ming and S. Nordholm, Quantum chemical exploration of the HCl dimer interaction 220 (1997) 63

- Mertz, E.L., E.D. German and A.M. Kuznetsov, Calculation of the solvent reorganization free energy in the dielectric cavity model 215 (1997) 355
- Mets, Ü., J. Widengren and R. Rigler, Application of the antibunching in dye fluorescence: measuring the excitation rates in solution 218 (1997) 191
- Meyer, H., see Richter, A. 214 (1997) 321
- Michel-Beyerle, M.E., see Lossau, H. 213 (1996) 1
- Michinomae, M., see Oeda, Y. 213 (1996) 421
- Middelhoek, E.R., H. Zhang, J.W. Verhoeven and M. Glasbeek, Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution 211 (1996) 489
- Mikkelsen, K.V., see Minaev, B.F. 220 (1997) 79
- Miklavc, A., see Marković, N. 211 (1996) 277
- Miller, W.H., see Lehr, L. 214 (1997) 301
- Millié, P., see Germain, A. 219 (1997) 265
- Minaev, B.F., K.V. Mikkelsen and H. Ågren, Collision-induced electronic transitions in complexes between benzene and molecular oxygen 220 (1997) 79
- Ming, L., see Meredith, A.W. 220 (1997) 63
- Minoshima, K., see Abraham, E. 219 (1997) 73
- Mirbach, B., see Gorin, T. 217 (1997) 145
- Miret-Artés, S., see Buonomo, E. 218 (1997) 71
- Miyawaki, J., see Schmid, R.P. 218 (1997) 291
- Miyazaki, T., see Kumada, T. 212 (1996) 177
- Miyoshi, E., see Honjou, N. 212 (1996) 363
- Mizuno, K., see Oeda, Y. 213 (1996) 421
- Möbius, K., see Salikhov, K.M. 215 (1997) 23
- Mohr, J.-H., see Koper, M.T.M. 220 (1997) 95
- Moiseyev, N., see Althorpe, S.C. 217 (1997) 289
- Moncorgé, R., see Capobianco, J.A. 214 (1997) 329
- Monnerville, M. and J.-M. Robbe, Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances 211 (1996) 249
- Morgner, H., see Dietter, J. 220 (1997) 261
- Morillo, M., C. Denk and R.I. Cukier, Control of tunneling reactions with an external field in a four-level system: A general Redfield approach 212 (1996) 157
- Morillo, M., see Cukier, R.I. 217 (1997) 179
- Mortensen, O.S., see Svendsen, C. 215 (1997) 89
- Motohashi, K., H. Soshi, M. Ukai and S. Tsurubuchi, Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species 213 (1996) 369
- Motylewski, T., J. Najbar and M. Tachiya, Competitive electron transfers in model triad systems: continuum model approach 212 (1996) 193
- Msezane, A.Z., see Felfli, Z. 211 (1996) 325
- Mulero, A., see Cuadros, F. 218 (1997) 235
- Muller, J.M., D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen, The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film 211 (1996) 413
- Müller, T., see Richter, A. 214 (1997) 321
- Munichandraiah, N., see Ray, P.C. 211 (1996) 499
- Munn, R.W., see Eilmes, A. 214 (1997) 341
- Munn, R.W., Charge-transfer excitons in the dielectric theory of molecular crystals 215 (1997) 301

- Nadtochenko, V.A., see Brazgun, F.F. 211 (1996) 469
- Nagata, T., see Kanda, K. 218 (1997) 199
- Najbar, J., see Motylewski, T. 212 (1996) 193
- Nakanaga, T., see Jäckel, J.-G. 215 (1997) 291
- Nakanaga, T., see Schmid, R.P. 218 (1997) 291
- Narymbetov, B.Zh., see Kveder, V.V. 216 (1997) 407
- Naumkin, F.Y., The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside 213 (1996) 33
- Navarro, A., see Kearley, G.J. 216 (1997) 323
- Nee, J.B. and S. Hubinger, Pressure effects on the $\text{Cl}_2(\text{D}'-\text{A}')$ transition at 258 nm 211 (1996) 403
- Nelander, B., see Engdahl, A. 213 (1996) 333
- Nelander, B., see Kölm, J. 214 (1997) 313
- Nemukhin, A.V., see Grigorenko, B.L. 219 (1997) 161
- Neumann, M. and G.J. Kearley, Rotation/precession of NH_3 groups in Hofmann clathrates 215 (1997) 253
- Neumann, M., see Johnson, M.R. 215 (1997) 343
- Nicklass, A., see Leininger, T. 217 (1997) 19
- Nicolai, B., see Johnson, M.R. 215 (1997) 343
- Nielsen, M.J., see Svendsen, C. 215 (1997) 89
- Nikitin, E.E., see Rosenblum, I. 213 (1996) 243
- Nishi, O., see Oeda, Y. 213 (1996) 421
- Nonomura, Y., S. Igarashi, N. Yoshioka and H. Inoue, Spectroscopic properties of chlorophylls and their derivatives. Influence of molecular structure on the electronic state 220 (1997) 155
- Nordholm, S., see Marković, N. 211 (1996) 277
- Nordholm, S., see Börjesson, L.E.B. 212 (1996) 393
- Nordholm, S., see Meredith, A.W. 220 (1997) 63
- North, S.W., T.J. Sears, G.E. Hall and T. Suzuki, Comment on "energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm" 211 (1996) 515
- Nota, M., see Cerny, D. 216 (1997) 207
- Novoderezhkin, V.I. and A.P. Razjivin, The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria 211 (1996) 203
- Nunzi, J.-M., see Delysse, S. 219 (1997) 341
- Oberlé, J., see Abraham, E. 214 (1997) 409
- Oberlé, J., see Abraham, E. 219 (1997) 73
- Obrebski, A., T. Kaps and U. Cerny, Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam 212 (1996) 311
- O'Connor, C.S.S., N.C. Jones and S.D. Price, The formation and dissociation of the dinitrogen pentoxide dication 214 (1997) 131
- Oeda, Y., O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto, Exciton scattering, *k* selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence 213 (1996) 421
- Ohtsuki, Y., see Watanabe, Y. 217 (1997) 317
- O'Keeffe, F.J., see Ruth, A.A. 217 (1997) 83
- Okrasinski, W., see Cuadros, F. 218 (1997) 235

- Olney, T.N., G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan, Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique 218 (1997) 127
- Ong, P.P. and M.-M. Li, Monte Carlo simulation studies on the validity of the Gram-Charlier calculations of velocity distributions of Na⁺ swarm in neon gas 211 (1996) 115
- Orea, J.M., see Garay Salazar, M. 216 (1997) 365
- Orea, J.M., A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña, Reaction dynamics of the Ca(¹D₂, ³P_J) + CH₃I → CaI* + CH₃ system: chemiluminescence, energy disposal and product polarization 220 (1997) 337
- Oref, I., see Rosenblum, I. 213 (1996) 243
- Ōsawa, E., see Slanina, Z. 219 (1997) 193
- Ossipyan, Yu.A., see Kveder, V.V. 216 (1997) 407
- Pac, B., see Eilmes, A. 214 (1997) 341
- Paidarová, I., see Sauer, S.P.A. 214 (1997) 91
- Paladi, F.G., see Coropceanu, V.P. 219 (1997) 1
- Palmer, M.H., H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel, The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies 214 (1997) 191
- Paluch, M., P. Habdas, S.J. Rzoska and T. Schimpel, Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution 213 (1996) 483
- Pansu, R., see Laguitton-Pasquier, H. 212 (1996) 437
- Papp, G., see Gudowska-Nowak, E. 220 (1997) 125
- Parak, F., see Chang, I. 212 (1996) 221
- Paramonov, G.K., see Korolkov, M.V. 217 (1997) 341
- Parisel, O., M. Hanus and Y. Ellinger, Interstellar silicon-nitrogen chemistry. I. The microwave and the infrared signatures of the HSiN, HNSi, HSiNH₂, HNSiH₂ and HSiNH⁺ species 212 (1996) 331
- Parker, S., see Fillaux, F. 216 (1997) 281
- Parkinson, W.H., see Yoshino, K. 211 (1996) 387
- Parkinson, W.H., see Yoshino, K. 215 (1997) 429
- Parson, R.P., see Peng, G.S. 211 (1996) 17
- Passarini, F., see Bendazzoli, G.L. 215 (1997) 217
- Paszkiewicz, A., see Plonka, A. 212 (1996) 1
- Pathak, S.K., see Gianturco, F.A. 215 (1997) 227
- Pathak, S.K., see Gianturco, F.A. 215 (1997) 239
- Pavlychev, A.A., see Franke, R. 216 (1997) 243
- Pedersen, J.B., see Jørgensen, J.S. 211 (1996) 235
- Pei, Z.W., see Tanner, P.A. 215 (1997) 125
- Peng, G.S. and R.P. Parson, Selective rovibrational energy transfer: A classical trajectory study of collisional energy redistribution in methyl radical 211 (1996) 17
- Penzkofer, A., see Reindl, S. 211 (1996) 431
- Penzkofer, A., see Reindl, S. 213 (1996) 429
- Penzkofer, A., see Weigand, R. 220 (1997) 373
- Penzkofer, A., see Rotermund, F. 220 (1997) 385
- Perchard, J.P., see Coussan, S. 219 (1997) 221

- Peremans, A., see Coussan, S. 219 (1997) 221
- Pericou-Cayere, M., M. Gelize and A. Dargelos, Ab initio calculations of electronic spectra of H_2S and H_2S_2 214 (1997) 81
- Perrin, M.-Y., see Porshnev, P.I. 213 (1996) 111
- Persico, M., see Cattaneo, P. 214 (1997) 49
- Persico, M., see Romstad, D. 219 (1997) 21
- Pesce, L. and P. Saalfrank, "Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule-surface scattering 219 (1997) 43
- Petelenz, P., see Eilmes, A. 214 (1997) 341
- Peters, D.W., see DeWitt, M.J. 218 (1997) 211
- Petrella, G., L. Cassidei and F. Ciriaco, Disordered surfaces: a smoothed He-target scattering potential for metal atoms adsorbed on metal surfaces 216 (1997) 391
- Petrov, E.G., I.S. Tolokh, V.V. Gorbach and V. May, The magnetic field influence on bridge-assisted electron transfer 220 (1997) 249
- Pettersson, J.B.C., see Svanberg, M. 220 (1997) 137
- Pfeiffer, M., see Werncke, W. 216 (1997) 337
- Phan, M.Q. and H. Rabitz, Learning control of quantum-mechanical systems by laboratory identification of effective input-output maps 217 (1997) 389
- Phillips, J.C., Kohlrausch relaxation in electronic and molecular glasses 212 (1996) 41
- Pilar de Lara, M., see Buonomo, E. 218 (1997) 71
- Plato, M., see Salikhov, K.M. 215 (1997) 23
- Plonka, A. and A. Paszkiewicz, Phenomenological interpretation of kinetics with time-dependent specific reaction rates 212 (1996) 1
- Pollacchi, A., see Palmer, M.H. 214 (1997) 191
- Pöllinger-Dammer, F., see Lossau, H. 213 (1996) 1
- Ponterini, G., Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis-trans photoisomerization dynamics 216 (1997) 193
- Popp, A., see Ujj, L. 212 (1996) 421
- Popp, A., see Ujj, L. 217 (1997) 115
- Porshnev, P.I., H.L. Wallaart, M.-Y. Perrin and J.-P. Martin, Modeling of optical pumping experiments in CO. I. Time-resolved experiments 213 (1996) 111
- Pouchan, C., see Maroulis, G. 215 (1997) 67
- Preuss, H., see Czuchaj, E. 214 (1997) 277
- Price, S.D., see O'Connor, C.S.S. 214 (1997) 131
- Probst, M., see Limtrakul, J. 215 (1997) 77
- Pulfer, M., C.-H. Hu and D.P. Chong, Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases 216 (1997) 91
- Quasso, F., see Consolati, G. 213 (1996) 449
- Rabitz, H., see Phan, M.Q. 217 (1997) 389
- Racine, S., see Coussan, S. 219 (1997) 221
- Raimond, P., see Delysse, S. 219 (1997) 341
- Raimondi, M., see Gianturco, F.A. 215 (1997) 227
- Raimondi, M., see Gianturco, F.A. 215 (1997) 239

- Randall, K.L. and D.J. Donaldson, Photophysics and photochemistry of I₂ (D, D') in rare gas clusters 211 (1996) 377
- Rapakoulas, D., see Stamou, S. 218 (1997) 57
- Ray, P.C., N. Munichandraiah and P.K. Das, Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques 211 (1996) 499
- Rayane, D., see Dugourd, Ph. 218 (1997) 163
- Raz, T. and R.D. Levine, Fast translational thermalization of extreme disequilibrium induced by cluster impact 213 (1996) 263
- Razjivin, A.P., see Novoderezhkin, V.I. 211 (1996) 203
- Rebentrost, F., see Czuchaj, E. 214 (1997) 277
- Reed, D., see Palmer, M.H. 214 (1997) 191
- Régis, A., see Fillaux, F. 216 (1997) 281
- Reid, K.L., see Wouters, E.R. 218 (1997) 309
- Reindl, S. and A. Penzkofer, Higher excited-state triplet-singlet intersystem crossing of some organic dyes 211 (1996) 431
- Reindl, S. and A. Penzkofer, Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation 213 (1996) 429
- Reinhardt, K., see Ahmed, M. 219 (1997) 333
- Reinhold, J., see Franke, R. 220 (1997) 299
- Reis, H. and W. Baumann, Influence of rotational diffusion on the electric field induced effect on the fluorescence spectrum of diluted solutions. I. Theory and numerical simulations 214 (1997) 383
- Renn, A., see Güttler, F. 211 (1996) 421
- Rennie, E.E., see Holland, D.M.P. 219 (1997) 91
- Rettig, W., see Maus, M. 218 (1997) 151
- Reuben, B.G., see Lukhezo, M. 220 (1997) 53
- Ribeiro, M.C.C., L.F.C. de Oliveira and P.S. Santos, Raman bandshape analysis of oxocarbon ions in aqueous solutions 217 (1997) 71
- Richard-Viard, M., see Dedonder-Lardeux, C. 212 (1996) 371
- Richter, A., H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig, Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study 214 (1997) 321
- Rickerby, A.G., see Green, N.J.B. 212 (1996) 99
- Rigler, R., see Widengren, J. 216 (1997) 417
- Rigler, R., see Mets, Ü. 218 (1997) 191
- Riley, M.J., see Wilson, C.R. 217 (1997) 63
- Rinaldi, C.A., see Orea, J.M. 220 (1997) 337
- Ring, S., see Eisenhardt, C.G. 216 (1997) 427
- Ripp, D.P., see Clark, B.K. 213 (1996) 229
- Rizzo, A., see Coriani, S. 216 (1997) 53
- Robbe, J.-M., see Monnerville, M. 211 (1996) 249
- Robinson, G.W., see Singh, S. 212 (1996) 125
- Rocchi, C., A.R. Bizzarri and S. Cannistraro, Water residence times around copper plastocyanin: a molecular dynamics simulation approach 214 (1997) 261
- Rode, B.M., see Kerdcharoen, T. 211 (1996) 313
- Rode, B.M., see Vizoso, S. 213 (1996) 77
- Rode, B.M., see Tongraar, A. 219 (1997) 279

- Røeggen, I., see Wind, P. 211 (1996) 179
- Rolke, J., Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy, Imaging of the HOMO electron density in $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ by electron momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations 215 (1997) 191
- Romstad, D., G. Granucci and M. Persico, Nonadiabatic transitions and interference in photodissociation dynamics 219 (1997) 21
- Rooyakkers, W.J.M., see Vredenbregt, E.J.D. 216 (1997) 259
- Rooyakkers, W.J.M., see Vredenbregt, E.J.D. 216 (1997) 273
- Rosenblum, I., E.I. Dashevskaya, E.E. Nikitin and I. Oref, On the sampling of microcanonical distribution for rotating triatomic molecules 213 (1996) 243
- Roston, G.D., M.S. Helmi and T. Grycuk, Interatomic potentials for XO^+ and B^3I states of intercombination cadmium line 326.1 nm broadened by Ar pressure 213 (1996) 365
- Rotermund, F., see Weigand, R. 220 (1997) 373
- Rotermund, F., R. Weigand and A. Penzkofer, J-aggregation and disaggregation of indocyanine green in water 220 (1997) 385
- Rozenberg, L.P., see Kveder, V.V. 216 (1997) 407
- Rubio, R.G., see Compostizo, A. 212 (1996) 301
- Rubtsov, I.V., see Brazgun, F.F. 211 (1996) 469
- Rüchardt, C., see Bensasson, R.V. 215 (1997) 111
- Rullière, C., see Abraham, E. 214 (1997) 409
- Rullière, C., see Abraham, E. 219 (1997) 73
- Ruth, A.A., F.J. O’Keeffe, R.P. Brint and M.W.D. Mansfield, The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione 217 (1997) 83
- Ruth, C., M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert, Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides 213 (1996) 454
- Ruud, K., see Coriani, S. 216 (1997) 53
- Ryabov, E.A., see Kosterev, A.A. 219 (1997) 305
- Rzoska, S.J., see Paluch, M. 213 (1996) 483
- Saalfrank, P., Stochastic wave packet vs. direct density matrix solution of Liouville–von Neumann equations for photodesorption problems 211 (1996) 265
- Saalfrank, P., see Pesce, L. 219 (1997) 43
- Sagarik, K. and P. Asawakun, Intermolecular potential for phenol based on the test particle model 219 (1997) 173
- Sagstuen, E., see Salih, N.A. 212 (1996) 409
- Saint-Espès, C., see Chapuisat, X. 217 (1997) 43
- Sakaguchi, Y., see Salikhov, K.M. 220 (1997) 355
- Sakai, K., A three-body calculation for collision-induced dissociation 220 (1997) 115
- Salih, N.A., O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen, Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR 212 (1996) 409
- Salikhov, K.M., J. Schlüpmann, M. Plato and K. Möbius, Calculation of triplet–singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs 215 (1997) 23
- Salikhov, K.M., Y. Sakaguchi and H. Hayashi, A contribution to the theory of OD EPR of spin-correlated radical pairs 220 (1997) 355

- Samanta, A. and S.K. Ghosh, A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates 214 (1997) 61
- Sansón, J.A., see Tolosa, S. 213 (1996) 203
- Sansone, R., see Limtrakul, J. 215 (1997) 77
- Santos, P.S., see Ribeiro, M.C.C. 217 (1997) 71
- Sapozhnikov, M.N., see Drobizhev, M.A. 211 (1996) 455
- Sarkar, P., S. Adhikari and S.P. Bhattacharyya, A quantal entropy signature for the dynamics of pure states: Studies on some model problems 215 (1997) 309
- Sastry, G.M., see Agmon, N. 212 (1996) 207
- Sauer, S.P.A., V. Špirko, I. Paidarová and W.P. Kraemer, The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH^- and $\text{OH}^- \cdot \text{H}_2\text{O}$ 214 (1997) 91
- Schael, F., J. Küster and H.-G. Löhmansröben, The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates 218 (1997) 175
- Scharnagl, C. and S.F. Fischer, Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model 212 (1996) 231
- Scheblykin, I.G., see Drobizhev, M.A. 211 (1996) 455
- Scheiner, S., see Latajka, Z. 216 (1997) 37
- Scherer, N.F., see Hayashi, M. 217 (1997) 259
- Schimpel, T., see Paluch, M. 213 (1996) 483
- Schinke, R., see Schwendner, P. 217 (1997) 233
- Schirmer, J., see Trofimov, A.B. 214 (1997) 153
- Schirrmeister, D.H. and V. May, Strong-field approach to ultrafast pump-probe spectra: dye molecules in solution 220 (1997) 1
- Schlüpmann, J., see Salikhov, K.M. 215 (1997) 23
- Schmickler, W., see Koper, M.T.M. 211 (1996) 123
- Schmickler, W., see Koper, M.T.M. 220 (1997) 95
- Schmid, R., see Jäckel, J.-G. 215 (1997) 291
- Schmid, R.P., P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones, Infrared spectroscopy of aniline-X ($\text{X} = \text{N}_2, \text{CH}_4, \text{CHF}_3, \text{CO}$) clusters and their corresponding cluster cations in the NH_2 -stretching vibration region 218 (1997) 291
- Schmidt, B., see Backhaus, P. 217 (1997) 131
- Schmidt, R.G., M.C. Böhm and J. Brickmann, Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters 215 (1997) 207
- Schmidtke, H.-H., see Biertümpel, I. 215 (1997) 271
- Schneider, F., see Gianturco, F.A. 211 (1996) 33
- Schouten, P.G., see Warman, J.M. 212 (1996) 183
- Schrems, O., see Kölm, J. 214 (1997) 313
- Schriver, A., see Bahou, M. 216 (1997) 105
- Schriver-Mazzuoli, L., see Bahou, M. 216 (1997) 105
- Schurath, U., see Tyczkowski, G. 215 (1997) 379
- Schweig, A., see Richter, A. 214 (1997) 321
- Schwendner, P., F. Seyl and R. Schinke, Photodissociation of Ar_2^+ in strong laser fields 217 (1997) 233
- Sears, T.J., see North, S.W. 211 (1996) 515
- Seidner, L., see Wolfseder, B. 217 (1997) 275

- Sewell, T.D., see Marković, N. 211 (1996) 277
Seyl, F., see Schwendner, P. 217 (1997) 233
Sgamellotti, A., see Zheng, Y. 212 (1996) 269
Shapiro, M., Z. Chen and P. Brumer, Simultaneous control of selectivity and yield of molecular dissociation. Pulsed incoherent interference control 217 (1997) 325
Sharafutdinov, R.G., see Belikov, A.E. 213 (1996) 319
Shaw, D.A., see Holland, D.M.P. 219 (1997) 91
Shen, S., see Durig, J.R. 213 (1996) 165
Shi, Y.Y., see Wan, S.Z. 211 (1996) 227
Shibaeva, R.P., see Kveder, V.V. 216 (1997) 407
Shkrob, I.A., see Tarasov, V.F. 212 (1996) 353
Shlesinger, M.F., see Zumofen, G. 212 (1996) 89
Shobatake, K., see Kanda, K. 218 (1997) 199
Shpinkova, L.G., see Holland, D.M.P. 219 (1997) 91
Shushin, A.I., see Jørgensen, J.S. 211 (1996) 235
Siebbeles, L.D.A., see Wouters, E.R. 218 (1997) 309
Siggel, M.R.F., see Palmer, M.H. 214 (1997) 191
Siggel, M.R.F., see Gingell, J.M. 220 (1997) 191
Silva, C.M., see Lossau, H. 213 (1996) 1
Singh, S. and G.W. Robinson, An analytical study of the Berezhkovskii-Pollak-Zitserman theory of rate processes in the critical region. II. The critical coupling plane 212 (1996) 125
Sinha, H.K., V.J. MacKenzie and R.P. Steer, Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes 213 (1996) 397
Sinicropi, J.A., J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger, Hole transport in vapor deposited enamines and enamine doped polymers 218 (1997) 331
Sipp, B., see Klein, G. 215 (1997) 131
Sironi, M., see Gianturco, F.A. 215 (1997) 227
Sironi, M., see Gianturco, F.A. 215 (1997) 239
Sjögren, L., see Götze, W. 212 (1996) 47
Slanina, Z., X. Zhao, S.-L. Lee and E. Ōsawa, C₉₀ temperature effects on relative stabilities of the IPR isomers 219 (1997) 193
Slavin, V.V., see Eremenko, V.V. 216 (1997) 1
Small, G.J., see Wu, H.-M. 218 (1997) 225
Smith, A.M., see Caspary, N. 220 (1997) 241
Smith, D., The tunneling frequencies of the isotopic forms of methane in rare-gas solids 220 (1997) 279
Smith, D.M., see Biehl, H. 214 (1997) 357
Smith, P., see Johnson, M.R. 215 (1997) 343
Smolinski, Z.J., see Clark, B.K. 213 (1996) 229
Snavey, D.L., see Mellouki, A. 220 (1997) 311
Sobolewski, A.L. and L. Adamowicz, An ab initio study of the potential energy surface in the S₁ state of 2-hydroxypyridine 213 (1996) 193
Solca, J., see Welker, M. 213 (1996) 253
Solgadi, D., see Dedonder-Lardeux, C. 212 (1996) 371
Song, J.-B. and E.A. Gislason, A theoretical test of the pairwise energy model for reactive cross sections 212 (1996) 259
Song, J.-B. and E.A. Gislason, Application of the pairwise energy model to various isotopic variations of the H + H₂ reaction 214 (1997) 23
Soshi, H., see Motohashi, K. 213 (1996) 369

- Sovkov, V.B., see Ivanov, V.S. 213 (1996) 295
- Spencer-Smith, R.D., see Green, N.J.B. 212 (1996) 99
- Špirko, V., see Sauer, S.P.A. 214 (1997) 91
- Spohr, E., see Kohlmeyer, A. 213 (1996) 211
- Sporleder, W., see Richter, A. 214 (1997) 321
- Sreedhara Rao, V. and A.K. Chandra, An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen 214 (1997) 103
- Stamou, S., D. Mataras and D. Rapakoulis, Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants 218 (1997) 57
- Standard, J.M., see Clark, B.K. 213 (1996) 229
- Steer, R.P., see Sinha, H.K. 213 (1996) 397
- Stefanovich, E.V., see Truong, T.N. 218 (1997) 31
- Steinebrunner, G., see Welker, M. 213 (1996) 253
- Steinman, E.A., see Kveder, V.V. 216 (1997) 407
- Steybe, F., F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann, Enhanced nonlinear optical properties and thermal stability of donor-acceptor substituted oligothiophenes 219 (1997) 317
- Stock, G., see Wolfseder, B. 217 (1997) 275
- Stockmann, R., see Tak, Y.-H. 212 (1996) 471
- Stoecklin, T., see Beghin, A. 215 (1997) 261
- Stoll, H., see Czuchaj, E. 214 (1997) 277
- Stoll, H., see Leininger, T. 217 (1997) 19
- Stone, E.G., see Canty, J.F. 216 (1997) 81
- Storozhev, A.V., A new method of calculating exponential operators for scattering problems 213 (1996) 313
- Storozhev, A.V., see Belikov, A.E. 213 (1996) 319
- Streubel, P., see Franke, R. 220 (1997) 299
- Sugawara, K., see Schmid, R.P. 218 (1997) 291
- Sumi, H., Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations 212 (1996) 9
- Suzuki, T., see North, S.W. 211 (1996) 515
- Svanberg, M., N. Marković and J.B.C. Pettersson, Scattering of large argon clusters from a Pt(111) surface with low collision velocities 220 (1997) 137
- Svendsen, C., M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark, A study of the 1B_2 excited state geometries of the metal-metal quadruply bonded compounds $Mo_2X_4(PMe_3)_4$ ($X = Cl, Br$ or I) 215 (1997) 89
- Svensson, S., see Enkvist, C. 214 (1997) 123
- Swiatla-Wojcik, D., see Hawlicka, E. 218 (1997) 49
- Syutkin, V.M. and V.A. Tolkachev, Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na_2O 212 (1996) 149
- Szargan, R., see Franke, R. 220 (1997) 299
- Szczepanski, J., S. Ekern, C. Chapo and M. Vala, Infrared spectroscopy of matrix-isolated carbon clusters, with emphasis on C_8 and C_9 211 (1996) 359
- Tabayashi, K., see Kanda, K. 218 (1997) 199
- Tachikawa, H., Dynamics of the vibrational mode-specific proton transfer reaction $NH_3^+(\nu_1) + NH_3 \rightarrow NH_2 + NH_4^+$: ab initio MO and classical trajectory studies 211 (1996) 305

- Tachiya, M., see Motylewski, T. 212 (1996) 193
- Tadjeddine, A., see Coussan, S. 219 (1997) 221
- Tajima, N., T. Taketsugu and K. Hirao, Theoretical study on adsorption and proton exchange reaction of H₂O on H-form zeolite 218 (1997) 257
- Tak, Y.-H., H. Vestweber, H. Bässler, A. Bleyer, R. Stockmann and H.-H. Hörhold, Time-resolved electroluminescence from single and bilayer LEDs based upon substituted poly-arylenevinylenes 212 (1996) 471
- Takeo, H., see Jäckel, J.-G. 215 (1997) 291
- Takeo, H., see Schmid, R.P. 218 (1997) 291
- Takeshima, M., see Oeda, Y. 213 (1996) 421
- Taketsugu, T., see Tajima, N. 218 (1997) 257
- Talbot, F., see Dedonder-Lardeux, C. 212 (1996) 371
- Tan, K.H., see Olney, T.N. 218 (1997) 127
- Tanner, P.A., J. Dexpert-Ghys, Z.W. Pei and J. Lin, Reported blue upconversion from U⁴⁺ doped into Cs₂ZrCl₆ single crystals under green laser excitation 215 (1997) 125
- Tanner, P.A., see Chua, M. 218 (1997) 83
- Tao, Y., see Xie, X. 213 (1996) 133
- Tarasov, V.F., H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob, Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence 212 (1996) 353
- Tardajos, G., see Orea, J.M. 220 (1997) 337
- Tarroni, R. and C. Zannoni, Order parameters and carbon shielding tensors of bis-MSB from ¹³C NMR measurements in a nematic liquid crystal 211 (1996) 337
- Tasumi, M., see Torii, H. 216 (1997) 67
- Teitelbaum, H., see Lifshitz, A. 219 (1997) 243
- Terzic, M., see Jovanovic-Kurepa, J. 211 (1996) 347
- Thompson, D.B., see Yench, A.J. 216 (1997) 227
- Tiukanov, A.S., see Belyaev, A.K. 220 (1997) 43
- Tol, A.J.W., Poly-amino-enolates: first examples of odd alternant conducting polymers 215 (1997) 319
- Tolkachev, V.A., see Syutkin, V.M. 212 (1996) 149
- Tolkachev, V.A., see Vyazovkin, V.L. 216 (1997) 135
- Tolokh, I.S., see Petrov, E.G. 220 (1997) 249
- Tolosa, S. and J.A. Sansón, Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde 213 (1996) 203
- Tomkinson, J., see Kearley, G.J. 216 (1997) 323
- Tong, X.-M. and S.-I. Chu, Theoretical study of multiple high-order harmonic generation by intense ultrashort pulsed laser fields: A new generalized pseudospectral time-dependent method 217 (1997) 119
- Tongraar, A., S. Hannongbua and B.M. Rode, Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia 219 (1997) 279
- Torii, H., M. Tasumi, I.M. Bell and R.J.H. Clark, Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn–Teller distortion in the excited electronic state on Raman intensities 216 (1997) 67
- Torop, L., see Jones, A.L. 211 (1996) 291
- Törning, J.T., see Knüpling, M. 219 (1997) 291
- Tran, V., see Leroux, B. 216 (1997) 349

- Treesukol, P., see Limtrakul, J. 215 (1997) 77
- Tremblay, B., M.E. Alikhani and L. Manceron, Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study 218 (1997) 37
- Trofimov, A.B. and J. Schirmer, Polarization propagator study of electronic excitation in key heterocyclic moleculesI. Pyrrole 214 (1997) 153
- Trommsdorff, H.P., see Benderskii, V.A. 219 (1997) 119
- Trommsdorff, H.P., see Benderskii, V.A. 219 (1997) 143
- Truong, T.N. and E.V. Stefanovich, Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential 218 (1997) 31
- Truscott, T.G., see Bensasson, R.V. 215 (1997) 111
- Tsurubuchi, S., see Motohashi, K. 213 (1996) 369
- Tuckett, R.P., see Biehl, H. 214 (1997) 357
- Tuckett, R.P., see Biehl, H. 214 (1997) 367
- Tyczkowski, G., U. Schurath, M. Bodenbinder and H. Willner, Matrix-isolated oxygen: line-shapes and transition probabilities of the $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$, $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ and $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transitions 215 (1997) 379
- Tyutyulkov, N., see Dietz, F. 218 (1997) 43
- Ujj, L., F. Jäger, A. Popp and G.H. Atkinson, Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy 212 (1996) 421
- Ujj, L., F. Jäger, A. Popp and G.H. Atkinson, Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Stokes Raman spectroscopy. [Chem. Phys. 212 (1996) 421-436] 217 (1997) 115
- Ukai, M., see Motohashi, K. 213 (1996) 369
- Umeda, H., see Watanabe, Y. 217 (1997) 317
- Un, S., see Knüpling, M. 219 (1997) 291
- Vala, M., see Szczepanski, J. 211 (1996) 359
- Valencia, E., see Cortés, J. 219 (1997) 235
- Van Amerongen, H., see Visser, H.M. 215 (1997) 299
- Van de Hurk, P.J., see Vredenbregt, E.J.D. 216 (1997) 259
- Van de Hurk, P.J., see Vredenbregt, E.J.D. 216 (1997) 273
- Van der Auweraer, M., see Drobizhev, M.A. 211 (1996) 455
- Van der Zande, W.J., see Wouters, E.R. 218 (1997) 309
- Van Faassen, E.E., see Muller, J.M. 211 (1996) 413
- Van Gerwen, R.J.F., see Vredenbregt, E.J.D. 216 (1997) 259
- Van Ginkel, G., see Muller, J.M. 211 (1996) 413
- Van Grondelle, R., see Visser, H.M. 215 (1997) 299
- Van Stokkum, I.H.M., see Visser, H.M. 215 (1997) 299
- Varandas, A.J.C. and W. Wang, On the $O_2(v') + O_2(v'')$ atmospheric reaction: a quasiclassical trajectory study 215 (1997) 167
- Varnavsky, O.P., see Drobizhev, M.A. 211 (1996) 455
- Varret, F., J. Linares and K. Boukheddaden, A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability 212 (1996) 487
- Varret, F., see Boukheddaden, K. 216 (1997) 373

- Veret-Lemarinier, A.V., see Kulikov, S.G. 216 (1997) 147
- Veret-Lemarinier, A.V., see Arabei, S.M. 216 (1997) 163
- Verhagen, J.C.D., see Muller, J.M. 211 (1996) 413
- Verhoeven, J.W., see Middelhoek, E.R. 211 (1996) 489
- Verrall, M.S., see Lukhezo, M. 220 (1997) 53
- Vervloet, M., see Dedonder-Lardeux, C. 212 (1996) 371
- Vestweber, H., see Tak, Y.-H. 212 (1996) 471
- Vetoshkin, E.V., see Benderskii, V.A. 219 (1997) 119
- Vetoshkin, E.V., see Benderskii, V.A. 219 (1997) 143
- Viehland, L.A., A.S. Dickinson and R.G.A.R. MacLagan, Transport coefficients for NO^+ ions in helium gas: a test of the NO^+ –He interaction potential 211 (1996) 1
- Villaeys, A.A., see Klein, G. 215 (1997) 131
- Villarreal, P., see Buonomo, E. 218 (1997) 71
- Vinogradov, S.A., see Brunel, M. 218 (1997) 301
- Visser, H.M., F.J. Kleima, I.H.M. van Stokkum, R. van Grondelle and H. van Amerongen, Probing the many energy-transfer processes in the photosynthetic light-harvesting complex II at 77 K using energy-selective sub-picosecond transient absorption spectroscopy (Chem. Phys. 210 (1996) 297–312) 215 (1997) 299
- Vitukhnovsky, A.G., see Drobizhev, M.A. 211 (1996) 455
- Vizoso, S. and B.M. Rode, Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures 213 (1996) 77
- Vojtík, J. and J. Fišer, Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+ 218 (1997) 13
- Von Busch, F., see Ankerhold, U. 220 (1997) 393
- Von Laue, L., see Benderskii, V.A. 219 (1997) 119
- Von Laue, L., see Benderskii, V.A. 219 (1997) 143
- Von Nagy-Felsobuki, E.I., see Hughes, J.M. 211 (1996) 135
- Von Niessen, W., see Zheng, Y. 212 (1996) 269
- Vredenbregt, E.J.D., W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck, Fine-structure dependence of the $\text{Ar}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer process 216 (1997) 259
- Vredenbregt, E.J.D., W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck, $\text{Ar}^*(^3\text{P}_2)/\text{Kr}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer collisions: final state rotational alignment 216 (1997) 273
- Vugts, M.J.M., see Vredenbregt, E.J.D. 216 (1997) 273
- Vyazovkin, V.L. and V.A. Tolkathev, Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives 216 (1997) 135
- Waliszewska, G., see Kolodziejski, M. 213 (1996) 341
- Walker, I.C., see Palmer, M.H. 214 (1997) 191
- Walker, I.C., see Gingell, J.M. 220 (1997) 191
- Wallaart, H.L., see Porshnev, P.I. 213 (1996) 111
- Waluk, J., see Dobrin, S. 216 (1997) 179
- Wan, S.Z., C.X. Wang, Y.W. Xu and Y.Y. Shi, Molecular dynamics simulations of cis–trans isomerization for a proline-containing tripeptide in solution 211 (1996) 227
- Wang, C.X., see Wan, S.Z. 211 (1996) 227
- Wang, D., see Wilson, C.R. 217 (1997) 63

- Wang, H. and W.L. Hase, Reaction path Hamiltonian analysis of the dynamics for $\text{Cl}^- + \text{CH}_3\text{Br} \rightarrow \text{ClCH}_3 + \text{Br}^-$ $\text{S}_\text{N}2$ nucleophilic substitution 212 (1996) 247
- Wang, H. and A.L. Cooksy, Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O 213 (1996) 139
- Wang, J., see Zheng, H. 211 (1996) 507
- Wang, W., see Varandas, A.J.C. 215 (1997) 167
- Wang, Y.-X. and C.-H. Deng, The formalism and matrix elements of a complete potential-harmonic scheme for directly solving the Schrödinger equation of the helium atom 214 (1997) 33
- Wannberg, B., see Eland, J.H.D. 212 (1996) 457
- Wannberg, B., see Holland, D.M.P. 219 (1997) 91
- Warman, J.M., P.G. Schouten, G.H. Gelinck and M.P. de Haas, The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines 212 (1996) 183
- Watanabe, Y., H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura, A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables 217 (1997) 317
- Weigand, R., F. Rotermund and A. Penzkofer, Degree of aggregation of indocyanine green in aqueous solutions determined by Mie scattering 220 (1997) 373
- Weigand, R., see Rotermund, F. 220 (1997) 385
- Weigold, E., see Zheng, Y. 212 (1996) 269
- Weiss, U., see Winterstetter, M. 217 (1997) 155
- Welker, M., G. Steinebrunner, J. Solca and H. Huber, Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 213 (1996) 253
- Werncke, W., M. Pfeiffer, T. Johr, A. Lau, W. Grahn, H.-H. Johannes and L. Dähne, Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines 216 (1997) 337
- Werner, H.-J., see Leininger, T. 217 (1997) 19
- Whitehead, J.C., see Ahmed, M. 219 (1997) 333
- Widengren, J., J. Dapprich and R. Rigler, Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy 216 (1997) 417
- Widengren, J., see Mets, Ü. 218 (1997) 191
- Wight, C.A., see Logan, D. 217 (1997) 99
- Wild, U.P., see Güttler, F. 211 (1996) 421
- Willart, J.F., see Delcourt, O. 215 (1997) 51
- Willner, H., see Tyczkowski, G. 215 (1997) 379
- Wilson, C.R., M.J. Riley, D. Wang and G.R. Hanson, Electron paramagnetic resonance of Ni(II) doped tris(ethylenediamine)zinc(II) dinitrate 217 (1997) 63
- Wind, P. and I. Røeggen, Ab initio calculation of three-body interaction in the $(\text{H}_2)_3$ trimer 211 (1996) 179
- Winterbottom, F., see Ahmed, M. 219 (1997) 333
- Winterstetter, M. and U. Weiss, Dynamical simulation of the driven spin-boson system: The influence of interblip correlations 217 (1997) 155
- Witschel, W., see Kohlmeyer, A. 213 (1996) 211
- Wolfseder, B., L. Seidner, G. Stock and W. Domcke, Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach 217 (1997) 275
- Wortmann, R., see Steybe, F. 219 (1997) 317
- Wouters, E.R., L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande, Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2 218 (1997) 309

- Wright, T.G., see Mack, P. 218 (1997) 243
- Wu, G., The anharmonic effect as originated from the asymmetry of a rotor. The case study of an asymmetric rotor coupled with a simple harmonic oscillator 214 (1997) 15
- Wu, H.-M. and G.J. Small, Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores 218 (1997) 225
- Wurfel, B.E., see Caspary, N. 220 (1997) 241
- Xie, X., Y. Tao, H. Cao and W. Duang, Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid 213 (1996) 133
- Xu, Y.W., see Wan, S.Z. 211 (1996) 227
- Yamaguchi, Y., see Matsushita, Y. 213 (1996) 413
- Yan, Y.J., J. Che and J.L. Krause, Optimal pump-dump control 217 (1997) 297
- Yang, B., see Guan, D. 218 (1997) 1
- Yang, M.M., see Lossau, H. 213 (1996) 1
- Yang, S., see Hu, Y. 218 (1997) 325
- Yang, T.-S., see Hayashi, M. 217 (1997) 259
- Yashiro, H., see Tarasov, V.F. 212 (1996) 353
- Yassar, A., see Klein, G. 215 (1997) 131
- Yencha, A.J., see Cormack, A.J. 213 (1996) 439
- Yencha, A.J., D.B. Thompson, A.J. Cormack, D.R. Cooper, M. Zubek, P. Bolognesi and G.C. King, Threshold photoelectron spectroscopy of SF₆ 216 (1997) 227
- Yi, X., see Guan, D. 218 (1997) 1
- Yoshino, K., J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui, Absorption cross section measurements of water vapor in the wavelength region 120 to 188 nm 211 (1996) 387
- Yoshino, K., J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui, Absorption cross section measurements of water vapor in the wavelength region 120 nm to 188 nm (Chem. Phys. 211 (1996) 387-391) 215 (1997) 429
- Yoshioka, N., see Nonomura, Y. 220 (1997) 155
- Youvan, D.C., see Lossau, H. 213 (1996) 1
- Yu, L.T., see Fillaux, F. 216 (1997) 281
- Yu, X.P., Z.L. Cao and R.S. Han, Hybridizations of fullerenes: their relations with properties and applications in computation 215 (1997) 1
- Zachariasse, K.A., see Il'ichev, Yu.V. 211 (1996) 441
- Zanardi, E.M. and J.M. Gomez Llorente, Dynamical resonance and tunneling in a driven system with periodic potential 217 (1997) 221
- Zannoni, C., see Tarroni, R. 211 (1996) 337
- Zhang, H., see Middelhoeck, E.R. 211 (1996) 489
- Zhang, J. and M. Baumgarten, Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I 214 (1997) 291
- Zhang, Q., see Zheng, H. 211 (1996) 507
- Zhang, Y., Photoacoustic spectra of BaFBr:Eu²⁺ phosphors 219 (1997) 353
- Zhao, H., see Gingell, J.M. 220 (1997) 191
- Zhao, K., see Zheng, Y. 212 (1996) 269
- Zhao, W., see Durig, J.R. 213 (1996) 165
- Zhao, X., see Slanina, Z. 219 (1997) 193
- Zharikov, A., see Chang, I. 212 (1996) 221

- Zheng, H., K. Jiang, Q. Zhang and J. Wang, Solvent effects on sol-gel transition of alginate solutions by addition of cupric ions 211 (1996) 507
- Zheng, W.Q., see Coussan, S. 219 (1997) 221
- Zheng, Y., C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen, Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine 212 (1996) 269
- Zheng, Y., see Rolke, J. 215 (1997) 191
- Zhou, L., see Durig, J.R. 213 (1996) 165
- Ziegeler, L., see Ruth, C. 213 (1996) 454
- Zilker, S.J. and D. Haarer, Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects 220 (1997) 167
- Zolotov, B., see Fainberg, B.D. 216 (1997) 7
- Zubek, M., see Yench, A.J. 216 (1997) 227
- Zuhrt, C., see Chapuisat, X. 217 (1997) 43
- Zülicke, L., see Chapuisat, X. 217 (1997) 43
- Zumofen, G., J. Klafter and M.F. Shlesinger, Reactions controlled by enhanced diffusion: Deterministic and stochastic approaches 212 (1996) 89

The first of these is the fact that the world is a very complex place and that the information needs of individuals and organisations are constantly changing. This means that the information services that we provide must be able to adapt to these changes. The second is the fact that the information services that we provide must be able to provide a high level of quality and reliability. This means that we must have a strong commitment to excellence in all that we do. The third is the fact that the information services that we provide must be able to provide a high level of customer service. This means that we must have a strong commitment to our customers and to their needs.

The fourth is the fact that the information services that we provide must be able to provide a high level of security. This means that we must have a strong commitment to the protection of our customers' information. The fifth is the fact that the information services that we provide must be able to provide a high level of flexibility. This means that we must be able to adapt to the changing needs of our customers. The sixth is the fact that the information services that we provide must be able to provide a high level of innovation. This means that we must be able to develop new and innovative ways of providing information services.

The seventh is the fact that the information services that we provide must be able to provide a high level of cost-effectiveness. This means that we must be able to provide our services at a reasonable cost. The eighth is the fact that the information services that we provide must be able to provide a high level of sustainability. This means that we must be able to provide our services in a way that is sustainable for the long term. The ninth is the fact that the information services that we provide must be able to provide a high level of transparency. This means that we must be able to provide our services in a way that is transparent to our customers.

The tenth is the fact that the information services that we provide must be able to provide a high level of accountability. This means that we must be able to provide our services in a way that is accountable to our customers. The eleventh is the fact that the information services that we provide must be able to provide a high level of integrity. This means that we must be able to provide our services in a way that is integrity to our customers. The twelfth is the fact that the information services that we provide must be able to provide a high level of honesty. This means that we must be able to provide our services in a way that is honesty to our customers.

The thirteenth is the fact that the information services that we provide must be able to provide a high level of fairness. This means that we must be able to provide our services in a way that is fairness to our customers. The fourteenth is the fact that the information services that we provide must be able to provide a high level of respect. This means that we must be able to provide our services in a way that is respect to our customers. The fifteenth is the fact that the information services that we provide must be able to provide a high level of compassion. This means that we must be able to provide our services in a way that is compassion to our customers.

The sixteenth is the fact that the information services that we provide must be able to provide a high level of empathy. This means that we must be able to provide our services in a way that is empathy to our customers. The seventeenth is the fact that the information services that we provide must be able to provide a high level of understanding. This means that we must be able to provide our services in a way that is understanding to our customers. The eighteenth is the fact that the information services that we provide must be able to provide a high level of tolerance. This means that we must be able to provide our services in a way that is tolerance to our customers.

The nineteenth is the fact that the information services that we provide must be able to provide a high level of patience. This means that we must be able to provide our services in a way that is patience to our customers. The twentieth is the fact that the information services that we provide must be able to provide a high level of kindness. This means that we must be able to provide our services in a way that is kindness to our customers. The twenty-first is the fact that the information services that we provide must be able to provide a high level of generosity. This means that we must be able to provide our services in a way that is generosity to our customers.

Subject index to volume 211–220

Methods

Theoretical

Group theory and algebras

- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF),
E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- The *d*-dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals
and alternative Sturmian basis sets, V. Aquilanti, S. Cavalli and C. Coletti 214 (1997) 1
- The anharmonic effect as originated from the asymmetry of a rotor. The case study of an
asymmetric rotor coupled with a simple harmonic oscillator, G. Wu 214 (1997) 15
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a
molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on
cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
- Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic
properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

Classical mechanics

- Transport coefficients for NO⁺ ions in helium gas: a test of the NO⁺–He interaction
potential, L.A. Viehland, A.S. Dickinson and R.G.A.R. MacLagan 211 (1996) 1
- Selective rovibrational energy transfer: A classical trajectory study of collisional energy
redistribution in methyl radical, G.S. Peng and R.P. Parson 211 (1996) 17
- Reaction path Hamiltonian analysis of the dynamics for Cl[−] + CH₃Br → ClCH₃ + Br[−]
S_N2 nucleophilic substitution, H. Wang and W.L. Hase 212 (1996) 247
- A theoretical test of the pairwise energy model for reactive cross sections, J.-B. Song and
E.A. Gislason 212 (1996) 259
- Application of the pairwise energy model to various isotopic variations of the H + H₂
reaction, J.-B. Song and E.A. Gislason 214 (1997) 23
- On the O₂(*v'*) + O₂(*v''*) atmospheric reaction: a quasiclassical trajectory study, A.J.C.
Varandas and W. Wang 215 (1997) 167
- Isotope effects on the rate constants for the processes O₂ + O → O + O₂ and O₂ + O + Ar
→ O₃ + Ar. On a modified ground-state potential energy surface for ozone, A. Gross
and G.D. Billing 217 (1997) 1

- Phase-space localization and level spacing distributions for a driven rotor with mixed regular/chaotic dynamics, T. Gorin, H.J. Korsch and B. Mirbach 217 (1997) 145
- Ultracold atoms in modulated standing light waves, K. Drese and M. Holthaus 217 (1997) 201
- Many body and quasiparticle approaches*
- Correlated electronic potential-energy surfaces for proton interactions with N₂, F.A. Gianturco, S. Kumar and F. Schneider 211 (1996) 33
- Reactions controlled by enhanced diffusion: Deterministic and stochastic approaches, G. Zumofen, J. Klafter and M.F. Shlesinger 212 (1996) 89
- Recovering boundaries for partly diffusion-controlled reaction kinetics, N.J.B. Green, R.D. Spencer-Smith and A.G. Rickerby 212 (1996) 99
- Control of tunneling reactions with an external field in a four-level system: A general Redfield approach, M. Morillo, C. Denk and R.I. Cukier 212 (1996) 157
- Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine, Y. Zheng, C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen 212 (1996) 269
- The ArCIF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- The formalism and matrix elements of a complete potential-harmonic scheme for directly solving the Schrödinger equation of the helium atom, Y.-X. Wang and C.-H. Deng 214 (1997) 33
- Polarization propagator study of electronic excitation in key heterocyclic molecules I. Pyrrole, A.B. Trofimov and J. Schirmer 214 (1997) 153
- Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state, P. Karafiloglou 214 (1997) 171
- Hybridizations of fullerenes: their relations with properties and applications in computation, X.P. Yu, Z.L. Cao and R.S. Han 215 (1997) 1
- Double exchange in distorted trimeric mixed-valence clusters, M.I. Belinsky 215 (1997) 7
- Theoretical study of the low-lying excited states of ABCO, DABCO and homologous cage amines, V. Galasso 215 (1997) 183
- Charge-transfer excitons in the dielectric theory of molecular crystals, R.W. Munn 215 (1997) 301
- Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235
- Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1
- Strong-field approach to ultrafast pump-probe spectra: dye molecules in solution, D.H. Schirrmeister and V. May 220 (1997) 1
- Highly correlated QDPT-CI calculations of valence and core photoelectron spectra of Ne, G. Fronzoni and P. Decleva 220 (1997) 15
- Coupling schemes and perturbative treatments*
- Solvent reorganization energy of electron transfer in weakly polar solvents, D.V. Matyushov 211 (1996) 47
- Spin-orbit effects in fullerenes, F.J. Adrian 211 (1996) 73
- Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations, H. Sumi 212 (1996) 9

- Irreversible random transition theory as applied to rate processes in condensed media:
 Transient effects of constrained configuration rearrangements in complex systems,
 Yu.A. Berlin 212 (1996) 29
- Spin–spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- The d -dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals
 and alternative Sturmian basis sets, V. Aquilanti, S. Cavalli and C. Coletti 214 (1997) 1
- Ab initio determination of quasi-diabatic states for multiple reaction pathways, P. Cattaneo
 and M. Persico 214 (1997) 49
- Ultracold atoms in modulated standing light waves, K. Drese and M. Holthaus 217 (1997) 201
- Dynamical resonance and tunneling in a driven system with periodic potential, E.M.
 Zanardi and J.M. Gomez Llorente 217 (1997) 221
- Photodissociation of Ar_2^+ in strong laser fields, P. Schwendner, F. Seyl and R. Schinke 217 (1997) 233
- Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed
 phases, M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer 217 (1997) 259
- Optimal pump-dump control, Y.J. Yan, J. Che and J.L. Krause 217 (1997) 297
- Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic
 properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1
- Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G.
 Granucci and M. Persico 219 (1997) 21
- Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by
 Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
- “Free” nuclear density propagation in two dimensions. The coupled-channel density
 matrix method and its application to inelastic molecule–surface scattering, L. Pesce and
 P. Saalfrank 219 (1997) 43
- Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton
 approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and
 H.P. Trommsdorff 219 (1997) 119
- Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A.
 Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143
- Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy
 surfaces: van der Waals complexes of He-Cl_2 and Ar-Cl_2 , B.L. Grigorenko, A.V.
 Nemukhin and V.A. Apkarian 219 (1997) 161
- Phenomenological model for reaction kinetics coupled to a relaxing environment, Y.A.
 Berlin, A.L. Burin and S.F. Fischer 220 (1997) 25

Relativistic quantum mechanics

- Imaging of the HOMO electron density in $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ by electron
 momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations, J.
 Rolke, Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy 215 (1997) 191
- Spin–orbit interaction in heavy group 13 atoms and TlAr , T. Leininger, A. Berning, A.
 Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad 217 (1997) 19

Transport quantum mechanics

- Universality of anomalous diffusion in extremely disordered systems, J.C. Dyre and J.M.
 Jacobsen 212 (1996) 61
- Remote ionization and recombination through the multichannel electron transfer, A.I.
 Burshtein and P.A. Frantsuzov 212 (1996) 137

- Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model, C. Scharnagl and S.F. Fischer 212 (1996) 231
- A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates, A. Samanta and S.K. Ghosh 214 (1997) 61
- Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA, V.V. Eremenko, V.A. Karachevtsev and V.V. Slavin 216 (1997) 1
- Dynamical simulation of the driven spin-boson system: The influence of interblip correlations, M. Winterstetter and U. Weiss 217 (1997) 155
- Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations, M. Grifoni, L. Hartmann and P. Hänggi 217 (1997) 167
- Control of tunneling processes with an external field in a four-level system: an analytic approach, R.I. Cukier, C. Denk and M. Morillo 217 (1997) 179
- Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases, M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer 217 (1997) 259
- Diatomics-in-molecules study of the ground and excited states of H_3^- , A.K. Belyaev and A.S. Tiukanov 220 (1997) 43
- The magnetic field influence on bridge-assisted electron transfer, E.G. Petrov, I.S. Tolokh, V.V. Gorbach and V. May 220 (1997) 249
- Equilibrium statistical mechanics*
- Solvent reorganization energy of electron transfer in weakly polar solvents, D.V. Matyushov 211 (1996) 47
- Al,Si ordering in chabazites: A Monte Carlo study, M.C. Gordillo and C.P. Herrero 211 (1996) 81
- Maximum entropy imaging and quantum molecular timescale generalized Langevin equation theory, H.K. McDowell and A.M. Clogston 211 (1996) 91
- Temperature dependence of the density of an ionic micellar system near the critical point, A. Compostizo, C. Martín, R.G. Rubio and A. Crespo Colin 212 (1996) 301
- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates, A. Samanta and S.K. Ghosh 214 (1997) 61
- Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters, R.G. Schmidt, M.C. Böhm and J. Brickmann 215 (1997) 207
- Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
- C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
- Structure and dynamics at the surface of a concentrated aqueous solution of CsF, J. Dietter and H. Morgner 220 (1997) 261
- Statistical mechanics of stationary states*
- The Neel point for spin-transition systems: toward a two-step transition, H. Bolvin 211 (1996) 101
- An analytical study of the Berezhkovskii–Pollak–Zitserman theory of rate processes in the critical region. II. The critical coupling plane, S. Singh and G.W. Robinson 212 (1996) 125

- On the degrees of circularity for various kinds of polarized light in a nonpolar liquid mixture, D.J. Lee and K.-R. Kim 214 (1997) 183
- Calculation of triplet–singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs, K.M. Salikhov, J. Schlüpmann, M. Plato and K. Möbius 215 (1997) 23
- Drift velocity of ions in lighter gases in electric and magnetic fields, L. Ferrari and A. Carbognani 215 (1997) 37
- A quantal entropy signature for the dynamics of pure states: Studies on some model problems, P. Sarkar, S. Adhikari and S.P. Bhattacharyya 215 (1997) 309
- Statistical mechanical treatment of reactive solvent extraction, M. Lukhezo, L.J. Dunne, B.G. Reuben and M.S. Verrall 220 (1997) 53
- Non-equilibrium thermodynamic and hydrodynamic theories*
- Monte Carlo simulation studies on the validity of the Gram–Charlier calculations of velocity distributions of Na^+ swarm in neon gas, P.P. Ong and M.-M. Li 211 (1996) 115
- A Kramers reaction rate theory for electrochemical ion transfer reactions, M.T.M. Koper and W. Schmickler 211 (1996) 123
- Kohlrausch relaxation in electronic and molecular glasses, J.C. Phillips 212 (1996) 41
- Dissipation and fluctuation for a randomly kicked particle: Normal and anomalous diffusion, E. Barkai and V. Fleurov 212 (1996) 69
- Competitive electron transfers in model triad systems: continuum model approach, T. Motylewski, J. Najbar and M. Tachiya 212 (1996) 193
- Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam, A. Obrebski, T. Kaps and U. Cerny 212 (1996) 311
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates, A. Samanta and S.K. Ghosh 214 (1997) 61
- Peculiarities of the enthalpy relaxation of a glassy crystal, O. Delcourt, M. Descamps, J. Even, M. Bertault and J.F. Willart 215 (1997) 51
- Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing, B.D. Fainberg and B. Zolotov 216 (1997) 7
- Effect of strong excitation of the CO_2 asymmetric mode on transport properties, A. Chikhaoui and E.V. Kustova 216 (1997) 297
- Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations, M. Grifoni, L. Hartmann and P. Hänggi 217 (1997) 167
- Ab initio schemes for stationary properties*
- Correlated electronic potential-energy surfaces for proton interactions with N_2 , F.A. Gianturco, S. Kumar and F. Schneider 211 (1996) 33
- Ab initio calculations of the rovibrational states of He_2N^{2+} , J.M. Hughes and E.I. von Nagy-Felsobuki 211 (1996) 135
- Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives, A. Broo and A. Holmén 211 (1996) 147
- The dissociation energies of FeF, FeCl, and FeBr and their positive ions, C.W. Bauschlicher Jr. 211 (1996) 163

- Rydberg basis set effects on ab initio second hyperpolarizabilities of H_2 , C_6H_6 and CS_2 molecules, T. Hamada 211 (1996) 171
- Ab initio calculation of three-body interaction in the $(H_2)_3$ trimer, P. Wind and I. Røeggen 211 (1996) 179
- Comments on the mode coupling theory for structural relaxation, W. Götze and L. Sjögren 212 (1996) 47
- Interstellar silicon–nitrogen chemistry. I. The microwave and the infrared signatures of the $HSiN$, $HNSi$, $HSiNH_2$, $HNSiH_2$ and $HSiNH^+$ species, O. Parisel, M. Hanus and Y. Ellinger 212 (1996) 331
- Ab initio study on the electronic structure of the $4^2\Sigma^+$ and $5^2\Sigma^+$ excited states of CO^+ , N. Honjou and E. Miyoshi 212 (1996) 363
- Intracuster ion–molecule reactions induced by the synchrotron radiation in allyl bromide–ammonia clusters, C. Dedonder-Lardeux, C. Jouvet, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard 212 (1996) 371
- An ab initio perturbed ion study of structural properties of TiO_2 , SnO_2 and GeO_2 rutile lattices, A.C. Camargo, J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés 212 (1996) 381
- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123
- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- On the calculation of hydrogen NMR chemical shielding, D.B. Chesnut 214 (1997) 73
- Ab initio calculations of electronic spectra of H_2S and H_2S_2 , M. Pericou-Cayere, M. Gelize and A. Dargelos 214 (1997) 81
- The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH^- and $OH^- \cdot H_2O$, S.P.A. Sauer, V. Špirko, I. Paidarová and W.P. Kraemer 214 (1997) 91
- An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen, V. Sreedhara Rao and A.K. Chandra 214 (1997) 103
- Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium–water clusters, J.C. Contador, M.A. Aguilar and F.J.O. del Valle 214 (1997) 113
- The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel 214 (1997) 191
- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the $FCO + H_2 \rightarrow HFCO + H$ abstraction reaction, J.S. Francisco 214 (1997) 213
- Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations, J.W. Boughton, S. Kristyan and M.C. Lin 214 (1997) 219

- Ab initio calculations of S_1 excited state vibrational spectra of benzene, naphthalene and anthracene, G.S. Jas and K. Kuczera 214 (1997) 229
- Electronic charge density transfer along a constrained reaction path from a hydronium ion configuration into a hydrogen chemisorption state on Cu(100), An.M. Kuznetsov and W. Lorenz 214 (1997) 243
- Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region, A. Fahr, P. Hassanzadeh, B. Laszlo and R.E. Huie 215 (1997) 59
- Dipole polarizability and hyperpolarizability of FCN, ClCN, BrCN and ICN, G. Maroulis and C. Pouchan 215 (1997) 67
- Structures and potential energy surface of Faujasitic zeolite/water, J. Limtrakul, P. Treesukol, C. Ebner, R. Sansone and M. Probst 215 (1997) 77
- Interaction forces and energy transfer dynamics of LiH ($^1\Sigma^+$) and helium atoms. I. The ab initio evaluation of the lowest potential energy surface, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper 215 (1997) 227
- Poly-amino-enolates: first examples of odd alternant conducting polymers, A.J.W. Tol 215 (1997) 319
- Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra, A.M. Mebel and S.-H. Lin 215 (1997) 329
- Structure, energetics and vibrational spectra of dimers, trimers, and tetramers of HX ($X = Cl, Br, I$), Z. Latajka and S. Scheiner 216 (1997) 37
- Cotton–Mouton effect and shielding polarizabilities of ethylene: an MCSCF study, S. Coriani, A. Rizzo, K. Ruud and T. Helgaker 216 (1997) 53
- Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn–Teller distortion in the excited electronic state on Raman intensities, H. Torii, M. Tasumi, I.M. Bell and R.J.H. Clark 216 (1997) 67
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81
- Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree–Fock method, F.E. Jorge, E.V.R. de Castro and A.B.F. da Silva 216 (1997) 317
- Spin–orbit interaction in heavy group 13 atoms and TlAr, T. Leininger, A. Berning, A. Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad 217 (1997) 19
- Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree–Fock approximation, J.M. Luis, J. Martí, M. Duran and J.L. Andrés 217 (1997) 29
- A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces, W. Jakubetz and B.L. Lan 217 (1997) 375
- Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+ , J. Vojtík and J. Fišer 218 (1997) 13
- Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
- Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O, N_2$ and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243
- Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57

- Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
- Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
- C₉₀ temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
- Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl₂–ClO complexes, S. Aloisio and J.S. Francisco 219 (1997) 201
- Theoretical study of cyclic radicals NO_x ($x = 2-6$), Y. Li and S. Iwata 219 (1997) 209
- Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221
- Quantum chemical exploration of the HCl dimer interaction, A.W. Meredith, L. Ming and S. Nordholm 220 (1997) 63
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H. Ågren 220 (1997) 79
- Computational and simulation methods*
- Transport coefficients for NO⁺ ions in helium gas: a test of the NO⁺–He interaction potential, L.A. Viehland, A.S. Dickinson and R.G.A.R. MacLagan 211 (1996) 1
- Selective rovibrational energy transfer: A classical trajectory study of collisional energy redistribution in methyl radical, G.S. Peng and R.P. Parson 211 (1996) 17
- Al,Si ordering in chabazites: A Monte Carlo study, M.C. Gordillo and C.P. Herrero 211 (1996) 81
- Maximum entropy imaging and quantum molecular timescale generalized Langevin equation theory, H.K. McDowell and A.M. Clogston 211 (1996) 91
- The Neel point for spin-transition systems: toward a two-step transition, H. Bolvin 211 (1996) 101
- Potential energy curve of the X0⁺(¹Σ⁺) ground state of HgAr determined from A0⁺(³Π) → X0⁺ and B1(³Σ⁺) → X0⁺ fluorescence spectra, J. Koperski 211 (1996) 191
- The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria, V.I. Novoderezhkin and A.P. Razjivin 211 (1996) 203
- Experimental and theoretical study of the recombination reaction of FC(O)O radicals, A.E. Croce, C.J. Cobos and E. Castellano 211 (1996) 215
- Molecular dynamics simulations of cis–trans isomerization for a proline-containing tripeptide in solution, S.Z. Wan, C.X. Wang, Y.W. Xu and Y.Y. Shi 211 (1996) 227
- Magnetic field dependent yield of geminate radical pair recombination in micelles. Effect of intraradical spin lattice relaxation, J.S. Jørgensen, J.B. Pedersen and A.I. Shushin 211 (1996) 235
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- Stochastic wave packet vs. direct density matrix solution of Liouville–von Neumann equations for photodesorption problems, P. Saalfrank 211 (1996) 265
- An improved classical approach quantum encounter treatment of collision-induced vibrational energy transfer. Application to He + CO ($n_i = 1, 2$), N. Marković, T.D. Sewell, S. Nordholm and A. Miklavc 211 (1996) 277
- Phenomenological interpretation of kinetics with time-dependent specific reaction rates, A. Plonka and A. Paszkiewicz 212 (1996) 1
- Kohlrausch relaxation in electronic and molecular glasses, J.C. Phillips 212 (1996) 41

- Universality of anomalous diffusion in extremely disordered systems, J.C. Dyre and J.M. Jacobsen 212 (1996) 61
- Reactions controlled by enhanced diffusion: Deterministic and stochastic approaches, G. Zumofen, J. Klafter and M.F. Shlesinger 212 (1996) 89
- A temperature-dependent effective potential explains CO binding to myoglobin, N. Agmon and G.M. Sastry 212 (1996) 207
- Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy, I. Chang, H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak 212 (1996) 221
- Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model, C. Scharnagl and S.F. Fischer 212 (1996) 231
- Reaction path Hamiltonian analysis of the dynamics for $\text{Cl}^- + \text{CH}_3\text{Br} \rightarrow \text{ClCH}_3 + \text{Br}^-$ $\text{S}_\text{N}2$ nucleophilic substitution, H. Wang and W.L. Hase 212 (1996) 247
- Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence, V.F. Tarasov, H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob 212 (1996) 353
- An ab initio perturbed ion study of structural properties of TiO_2 , SnO_2 and GeO_2 rutile lattices, A.C. Camargo, J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés 212 (1996) 381
- Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203
- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Exploratory Pariser–Parr–Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- The formalism and matrix elements of a complete potential-harmonic scheme for directly solving the Schrödinger equation of the helium atom, Y.-X. Wang and C.-H. Deng 214 (1997) 33
- A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates, A. Samanta and S.K. Ghosh 214 (1997) 61
- On the calculation of hydrogen NMR chemical shielding, D.B. Chesnut 214 (1997) 73
- A new potential for the description of intermolecular interactions for rigid biaxial molecules, V.V. Ginzburg, M.A. Glaser and N.A. Clark 214 (1997) 253

- Water residence times around copper plastocyanin: a molecular dynamics simulation approach, C. Rocchi, A.R. Bizzarri and S. Cannistraro 214 (1997) 261
- Calculation of ground- and excited-state potential energy curves for the Hg_2 molecule in a pseudopotential approach, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 214 (1997) 277
- Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I, J. Zhang and M. Baumgarten 214 (1997) 291
- Hybridizations of fullerenes: their relations with properties and applications in computation, X.P. Yu, Z.L. Cao and R.S. Han 215 (1997) 1
- Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters, R.G. Schmidt, M.C. Böhm and J. Brickmann 215 (1997) 207
- Is He H^- a stable system?, G.L. Bendazzoli, S. Evangelisti and F. Passarini 215 (1997) 217
- The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid, M.R. Johnson, M. Neumann, B. Nicolai, P. Smith and G.J. Kearley 215 (1997) 343
- Calculation of the solvent reorganization free energy in the dielectric cavity model, E.L. Mertz, E.D. German and A. M. Kuznetsov 215 (1997) 355
- Cotton–Mouton effect and shielding polarizabilities of ethylene: an MCSCF study, S. Coriani, A. Rizzo, K. Ruud and T. Helgaker 216 (1997) 53
- Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn–Teller distortion in the excited electronic state on Raman intensities, H. Torii, M. Tasumi, I.M. Bell and R.J.H. Clark 216 (1997) 67
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases, M. Pulfer, C.-H. Hu and D.P. Chong 216 (1997) 91
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules, C.-H. Hu and D.P. Chong 216 (1997) 99
- Structure and selective visible photodissociation of the $\text{O}_3\text{:Br}_2$ and $\text{O}_3\text{:BrCl}$ complexes: an infrared matrix isolation and ab initio study, M. Bahou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 216 (1997) 105
- Orientational correlations in liquid carbon tetrabromide: a neutron diffraction and RMC study, I. Bakó, J.C. Dore and D.W. Huxley 216 (1997) 119
- Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine, G.J. Kearley, J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez 216 (1997) 323
- Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines, W. Werncke, M. Pfeiffer, T. Johr, A. Lau, W. Grahn, H.-H. Johannes and L. Dähne 216 (1997) 337
- Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose, B. Leroux, H. Bizot, J.W. Brady and V. Tran 216 (1997) 349
- Theoretical study of multiple high-order harmonic generation by intense ultrashort pulsed laser fields: A new generalized pseudospectral time-dependent method, X.-M. Tong and S.-I. Chu 217 (1997) 119
- Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury, P. Backhaus and B. Schmidt 217 (1997) 131
- Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach, B. Wolfseder, L. Seidner, G. Stock and W. Domcke 217 (1997) 275

- A time-independent wavepacket approach to the (t, t') -method for treating time-dependent Hamiltonian systems, S.C. Althorpe, D.J. Kouri, D.K. Hoffman and N. Moiseyev 217 (1997) 289
- A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables, Y. Watanabe, H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura 217 (1997) 317
- A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces, W. Jakubetz and B.L. Lan 217 (1997) 375
- Learning control of quantum-mechanical systems by laboratory identification of effective input–output maps, M.Q. Phan and H. Rabitz 217 (1997) 389
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulas 218 (1997) 57
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
- Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257
- Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
- C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
- Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy, J. Cortés and E. Valencia 219 (1997) 235
- The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
- Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
- Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
- Highly correlated QDPT-CI calculations of valence and core photoelectron spectra of Ne, G. Fronzoni and P. Decleva 220 (1997) 15
- Quantum effects in adiabatic electrochemical electron-transfer reactions, M.T.M. Koper, J.-H. Mohr and W. Schmickler 220 (1997) 95
- A three-body calculation for collision-induced dissociation, K. Sakai 220 (1997) 115
- Two-level system with noise: Blue's function approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 220 (1997) 125
- Structure and dynamics at the surface of a concentrated aqueous solution of CsF, J. Dietter and H. Morgner 220 (1997) 261
- The tunneling frequencies of the isotopic forms of methane in rare-gas solids, D. Smith 220 (1997) 279
- Classification of Cm I energy levels using PCA–BPN and PCA–NLM, X. Cao, H. Liu and N. Chen 220 (1997) 289

- Extended Fenske-Hall LCAO MO calculations of core-level shifts in solid P compounds, R. Franke, T. Chassé, J. Reinhold, P. Streubel and R. Szargan 220 (1997) 299
- Molecular dynamics and scattering theory*
- Spin-orbit effects in fullerenes, F.J. Adrian 211 (1996) 73
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- Stochastic wave packet vs. direct density matrix solution of Liouville-von Neumann equations for photodesorption problems, P. Saalfrank 211 (1996) 265
- An improved classical approach quantum encounter treatment of collision-induced vibrational energy transfer. Application to $\text{He} + \text{CO}$ ($n_i = 1, 2$), N. Marković, T.D. Sewell, S. Nordholm and A. Miklavc 211 (1996) 277
- An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region, A.L. Jones, A.J. Blake, L. Torop and D.G. McCoy 211 (1996) 291
- Translational spectroscopy of H^- produced by collision induced dissociation of H_3^+ on He, H. Martinez and A. Amaya-Tapia 211 (1996) 299
- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- A QM/MM simulation method applied to the solution of Li^+ in liquid ammonia, T. Kerdcharoen, K.R. Liedl and B.M. Rode 211 (1996) 313
- Generalized oscillator strengths for SF_6 in the S 2p inner-shell region, Z. Felfli, I. Fomunung, D. Bessis and A.Z. Msezane 211 (1996) 325
- Kohlrausch relaxation in electronic and molecular glasses, J.C. Phillips 212 (1996) 41
- Dynamic effects in non-adiabatic charge transfer, E. Gudowska-Nowak 212 (1996) 115
- Reaction path Hamiltonian analysis of the dynamics for $\text{Cl}^- + \text{CH}_3\text{Br} \rightarrow \text{ClCH}_3 + \text{Br}^-$ $\text{S}_\text{N}2$ nucleophilic substitution, H. Wang and W.L. Hase 212 (1996) 247
- A theoretical test of the pairwise energy model for reactive cross sections, J.-B. Song and E.A. Gislason 212 (1996) 259
- A partially ergodic multiple encounter theory of collisional energy transfer, L.E.B. Börjesson and S. Nordholm 212 (1996) 393
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- The anharmonic effect as originated from the asymmetry of a rotor. The case study of an asymmetric rotor coupled with a simple harmonic oscillator, G. Wu 214 (1997) 15

- Application of the pairwise energy model to various isotopic variations of the $\text{H} + \text{H}_2$ reaction, J.-B. Song and E.A. Gislason 214 (1997) 23
- A classical approach to resonant low-energy electron scattering off molecules: application to the a_1 -shape resonance of CF_3Cl , L. Lehr, J. Manz and W.H. Miller 214 (1997) 301
- A study of the $^1\text{B}_2$ excited state geometries of the metal–metal quadruply bonded compounds $\text{Mo}_2\text{X}_4(\text{PMe}_3)_4$ ($\text{X} = \text{Cl, Br or I}$), C. Svendsen, M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark 215 (1997) 89
- On the $\text{O}_2(\nu') + \text{O}_2(\nu'')$ atmospheric reaction: a quasiclassical trajectory study, A.J.C. Varandas and W. Wang 215 (1997) 167
- Imaging of the HOMO electron density in $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ by electron momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations, J. Rolke, Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy 215 (1997) 191
- Interaction forces and energy transfer dynamics of $\text{LiH}(^1\Sigma^+)$ and helium atoms. II. Rotationally inelastic collisions and excitation efficiency, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi and M. Sironi 215 (1997) 239
- Rotation/precession of NH_3 groups in Hofmann clathrates, M. Neumann and G.J. Kearley 215 (1997) 253
- The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory, A. Beghin and T. Stoecklin 215 (1997) 261
- Poly-amino-enolates: first examples of odd alternant conducting polymers, A.J.W. Tol 215 (1997) 319
- On the determination of $D_0^0(\text{CaBr})$ from translational energy threshold measurements, M. Garay Salazar, J.M. Orea and A. González Ureña 216 (1997) 365
- Vibronic theory of electric hysteresis in “bistable” mixed-valence molecular salts, K. Boukheddaden and F. Varret 216 (1997) 373
- Disordered surfaces: a smoothed He–target scattering potential for metal atoms adsorbed on metal surfaces, G. Petrella, L. Cassidei and F. Ciriaco 216 (1997) 391
- A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH , X. Chapuisat, C. Saint-Espès, C. Zuhrt and L. Zülicke 217 (1997) 43
- Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury, P. Backhaus and B. Schmidt 217 (1997) 131
- Phase-space localization and level spacing distributions for a driven rotor with mixed regular/chaotic dynamics, T. Gorin, H.J. Korsch and B. Mirbach 217 (1997) 145
- Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule, H. Dietz, A. Materny and V. Engel 217 (1997) 249
- A time-independent wavepacket approach to the (t, t') -method for treating time-dependent Hamiltonian systems, S.C. Althorpe, D.J. Kouri, D.K. Hoffman and N. Moiseyev 217 (1997) 289
- Optimal pump-dump control, Y.J. Yan, J. Che and J.L. Krause 217 (1997) 297
- Simultaneous control of selectivity and yield of molecular dissociation. Pulsed incoherent interference control, M. Shapiro, Z. Chen and P. Brumer 217 (1997) 325
- Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association, M.V. Korolkov, J. Manz and G.K. Paramonov 217 (1997) 341
- Learning control of quantum-mechanical systems by laboratory identification of effective input–output maps, M.Q. Phan and H. Rabitz 217 (1997) 389
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49

- A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $\text{Cs}_2\text{NaCeCl}_6$, M. Chua and P.A. Tanner 218 (1997) 83
- “Free” nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43
- Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279
- The relationship between the molecular structure of semiquinone radicals and their g -values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291
- Diatomics-in-molecules study of the ground and excited states of H_3^- , A.K. Belyaev and A.S. Tiukanov 220 (1997) 43
- Scattering of large argon clusters from a Pt(111) surface with low collision velocities, M. Svanberg, N. Marković and J.B.C. Pettersson 220 (1997) 137
- Structure and dynamics at the surface of a concentrated aqueous solution of CsF, J. Dietter and H. Morgner 220 (1997) 261
- Spectroscopic investigation of ground state pyrrole ($^{12}\text{C}_4\text{H}_5\text{N}$): the N–H stretch, A. Mellouki, R. Georges, M. Herman, D.L. Snively and S. Leytner 220 (1997) 311
- Forward and reverse excitation energy transport in concentrated two-component systems, P. Bojarski and L. Kułak 220 (1997) 323
- Reaction dynamics of the $\text{Ca}(^1\text{D}_2, ^3\text{P}_J) + \text{CH}_3\text{I} \rightarrow \text{CaI}^* + \text{CH}_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña 220 (1997) 337

Experimental

Magnetic resonances

- Order parameters and carbon shielding tensors of bis-MSB from ^{13}C NMR measurements in a nematic liquid crystal, R. Tarroni and C. Zannoni 211 (1996) 337
- Time evolution of the rate constant for the tunneling reaction $\text{H}_2 + \text{D} \rightarrow \text{H} + \text{HD}$ in solid D_2 – H_2 mixtures at very low temperature, T. Kumada, Y. Aratono and T. Miyazaki 212 (1996) 177
- Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR, N.A. Salih, O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen 212 (1996) 409
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- Calculation of triplet–singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs, K.M. Salikhov, J. Schlüpmann, M. Plato and K. Möbius 215 (1997) 23
- Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives, V.L. Vyazovkin and V.A. Tolkmachev 216 (1997) 135
- Electron paramagnetic resonance of Ni(II) doped tris(ethylenediamine)zinc(II) dinitrate, C.R. Wilson, M.J. Riley, D. Wang and G.R. Hanson 217 (1997) 63
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355

Cyclotron resonance

- Nonradiative processes and infrared emission in matrix isolated ND, N. Caspary, B.E. Wurfel, A.M. Smith and V.E. Bondybey 220 (1997) 241

Microwave spectroscopy

- Rotational and vibrational excitation of the N_2^+ (B) state in a He + N_2 electron-beam plasma, A.E. Belikov 215 (1997) 97
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267

Infrared spectroscopy

- Ab initio calculations of the rovibrational states of He_2N^{2+} , J.M. Hughes and E.I. von Nagy-Felsobuki 211 (1996) 135
- Multiple absorption and relaxation processes in SF_6-CH_4 mixtures: an experimental study, J. Jovanovic-Kurepa, D.D. Markusev and M. Terzic 211 (1996) 347
- Infrared spectroscopy of matrix-isolated carbon clusters, with emphasis on C_8 and C_9 , J. Szczepanski, S. Ekern, C. Chapo and M. Vala 211 (1996) 359
- Isotope effects in the photochemical formation of $HHgCH_3$ and $DHgCD_3$ in nitrogen and methane matrices, N. Legay-Sommaire and F. Legay 211 (1996) 367
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejski, G. Waliszewska and H. Abramczyk 213 (1996) 341
- A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices, J. Kölm, A. Engdahl, O. Schrems and B. Nelander 214 (1997) 313
- Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study, A. Richter, H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig 214 (1997) 321
- Spectroscopy and photophysics of $C_{60}H_{18}$ and $C_{60}H_{36}$, R.V. Bensasson, T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt 215 (1997) 111
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81
- Structure and selective visible photodissociation of the $O_3:Br_2$ and $O_3:BrCl$ complexes: an infrared matrix isolation and ab initio study, M. Bahou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 216 (1997) 105
- Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine, G.J. Kearley, J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez 216 (1997) 323
- Infrared bands of mass-selected carbon chains C_n ($n = 8-12$) and C_n^- ($n = 5-10, 12$) in neon matrices, P. Freivogel, M. Grutter, D. Forney and J.P. Maier 216 (1997) 401
- A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH, X. Chapuisat, C. Saint-Espès, C. Zuhrt and L. Züllicke 217 (1997) 43
- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37

- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- Infrared spectroscopy of aniline-X ($X = N_2, CH_4, CHF_3, CO$) clusters and their corresponding cluster cations in the NH_2 -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221
- Spectroscopic investigation of ground state pyrrole ($^{12}C_4H_5N$): the N-H stretch, A. Mellouki, R. Georges, M. Herman, D.L. Snively and S. Leytner 220 (1997) 311

Raman spectroscopy

- Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy, L. Ujj, F. Jäger, A. Popp and G.H. Atkinson 212 (1996) 421
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejewski, G. Waliszewska and H. Abramczyk 213 (1996) 341
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357
- A study of the 1B_2 excited state geometries of the metal-metal quadruply bonded compounds $Mo_2X_4(PMe_3)_4$ ($X = Cl, Br$ or I), C. Svendsen, M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark 215 (1997) 89
- Spectroscopy and photophysics of $C_{60}H_{18}$ and $C_{60}H_{36}$, R.V. Bensasson, T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt 215 (1997) 111
- Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn-Teller distortion in the excited electronic state on Raman intensities, H. Torii, M. Tasumi, I.M. Bell and R.J.H. Clark 216 (1997) 67
- Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine, G.J. Kearley, J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez 216 (1997) 323
- Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines, W. Werncke, M. Pfeiffer, T. Johr, A. Lau, W. Grahn, H.-H. Johannes and L. Dähne 216 (1997) 337
- Raman bandshape analysis of oxocarbon ions in aqueous solutions, M.C.C. Ribeiro, L.F.C. de Oliveira and P.S. Santos 217 (1997) 71
- Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83
- Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305

Visible and UV spectroscopy

- Potential energy curve of the $X0^+(^1\Sigma^+)$ ground state of $HgAr$ determined from $A0^+(^3\Pi) \rightarrow X0^+$ and $B1(^3\Sigma^+) \rightarrow X0^+$ fluorescence spectra, J. Koperski 211 (1996) 191
- An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region, A.L. Jones, A.J. Blake, L. Torop and D.G. McCoy 211 (1996) 291
- Photophysics and photochemistry of I_2 (D, D') in rare gas clusters, K.L. Randall and D.J. Donaldson 211 (1996) 377

- Absorption cross section measurements of water vapor in the wavelength region 120 to 188 nm, K. Yoshino, J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui 211 (1996) 387
- Fast-ion beam laser spectroscopy of $^{14}\text{N}_2^+$ and $^{15}\text{N}_2^+$: high-resolution study of the (1, 2) band of the $\text{B } ^2\Sigma_u^+ - \text{X } ^2\Sigma_g^+$ system, K. Boudjarane, A. Alikacem and M. Larzillière 211 (1996) 393
- Pressure effects on the $\text{Cl}_2(\text{D}' - \text{A}')$ transition at 258 nm, J.B. Nee and S. Hubinger 211 (1996) 403
- The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film, J.M. Muller, D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen 211 (1996) 413
- A temperature-dependent effective potential explains CO binding to myoglobin, N. Agmon and G.M. Sastry 212 (1996) 207
- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore–protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- Interatomic potentials for XO^+ and B^3I states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H}(\text{D}) + \text{N}_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385
- Polarization propagator study of electronic excitation in key heterocyclic molecules I. Pyrrole, A.B. Trofimov and J. Schirmer 214 (1997) 153
- The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel 214 (1997) 191
- A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices, J. Kölm, A. Engdahl, O. Schrems and B. Nelander 214 (1997) 313
- Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study, A. Richter, H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig 214 (1997) 321
- Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er^{3+} in YVO_4 , J.A. Capobianco, P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli 214 (1997) 329
- Charge-transfer states and the band gap in crystalline fullerene, A. Eilmes, R.W. Munn, B. Pac and P. Petelenz 214 (1997) 341
- Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution, S.A. Bagnich 214 (1997) 351
- Vacuum-UV fluorescence spectroscopy of CF_3X ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) in the range 10–30 eV, H. Biehl, K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims 214 (1997) 367
- Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region, A. Fahr, P. Hassanzadeh, B. Laszlo and R.E. Huie 215 (1997) 59
- A study of the $^1\text{B}_2$ excited state geometries of the metal–metal quadruply bonded compounds $\text{Mo}_2\text{X}_4(\text{PMe}_3)_4$ ($\text{X} = \text{Cl}, \text{Br}$ or I), C. Svendsen, M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark 215 (1997) 89
- Spectroscopy and photophysics of $\text{C}_{60}\text{H}_{18}$ and $\text{C}_{60}\text{H}_{36}$, R.V. Bensasson, T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt 215 (1997) 111

- Reported blue upconversion from U^{4+} doped into Cs_2ZrCl_6 single crystals under green laser excitation, P.A. Tanner, J. Dexpert-Ghys, Z.W. Pei and J. Lin 215 (1997) 125
- Sol-gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion, S.G. Kulikov, A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot 216 (1997) 147
- Sol-gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis, S.M. Arabei, S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup 216 (1997) 163
- Photophysics of *trans*-stilbene analogues: indolo[3,2-*b*]indole and its heterosubstituted sulfur and selenium derivatives, S. Dobrin, P. Kaszynski, S. Ikeda and J. Waluk 216 (1997) 179
- Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis-trans photoisomerization dynamics, G. Ponterini 216 (1997) 193
- Infrared bands of mass-selected carbon chains C_n ($n = 8-12$) and C_n^- ($n = 5-10, 12$) in neon matrices, P. Freivogel, M. Grutter, D. Forney and J.P. Maier 216 (1997) 401
- The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione, A.A. Ruth, F.J. O'Keeffe, R.P. Brint and M.W.D. Mansfield 217 (1997) 83
- Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulas 218 (1997) 57
- Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p, 2s; Cl 2p, 2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Reverse saturable absorption in palladium and zinc tetraphenyltetraenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301
- Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
- Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
- Enhanced nonlinear optical properties and thermal stability of donor-acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
- Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ ($XY \equiv FCl, Cl_2, FH$), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H. Ågren 220 (1997) 79
- Spectroscopic properties of chlorophylls and their derivatives. Influence of molecular structure on the electronic state, Y. Nonomura, S. Igarashi, N. Yoshioka and H. Inoue 220 (1997) 155

- Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects, S.J. Zilker and D. Haarer 220 (1997) 167
- Non-exponential decays of the S_1 vibronic levels of acetaldehyde, S.-H. Lee and I.-C. Chen 220 (1997) 175
- VUV optical-absorption and electron-energy-loss spectroscopy of formamide, J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel 220 (1997) 191
- The photoabsorption spectrum of vinylchloride (C_2H_3Cl) in the 8–12 eV range, R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 207
- Forward and reverse excitation energy transport in concentrated two-component systems, P. Bojarski and L. Kułak 220 (1997) 323
- Reaction dynamics of the $Ca(^1D_2, ^3P_J) + CH_3I \rightarrow CaI^* + CH_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña 220 (1997) 337
- J-aggregation and disaggregation of indocyanine green in water, F. Rotermund, R. Weigand and A. Penzkofer 220 (1997) 385
- Fluorescence spectroscopy*
- Pressure effects on the $Cl_2(D'-A')$ transition at 258 nm, J.B. Nee and S. Hubinger 211 (1996) 403
- The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film, J.M. Muller, D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen 211 (1996) 413
- Single molecule polarization spectroscopy: pentacene in p-terphenyl, F. Güttler, M. Croci, A. Renn and U.P. Wild 211 (1996) 421
- Higher excited-state triplet–singlet intersystem crossing of some organic dyes, S. Reindl and A. Penzkofer 211 (1996) 431
- Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans–cis photoisomerisation, Yu.V. Il'ichev, W. Kühnle and K.A. Zachariasse 211 (1996) 441
- The charge transfer state of excited bianthryl and a derivative: solvatochromism, emission CT spectra broadening in homogeneous solvents, H. Laguitton-Pasquier, R. Pansu, J.-P. Chauvet, A. Collet, J. Faure and R. Lapouyade 212 (1996) 437
- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore–protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- Photodissociation dynamics of $HN_3(DN_3) + h\nu \rightarrow H(D) + N_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone–carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429

- Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er^{3+} in YVO_4 , J.A. Capobianco, P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli 214 (1997) 329
- The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF_3X^+ ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) ions, H. Biehl, K.J. Boyle, D.M. Smith and R.P. Tuckett 214 (1997) 357
- Vacuum-UV fluorescence spectroscopy of CF_3X ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) in the range 10–30 eV, H. Biehl, K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims 214 (1997) 367
- Influence of rotational diffusion on the electric field induced effect on the fluorescence spectrum of diluted solutions. I. Theory and numerical simulations, H. Reis and W. Baumann 214 (1997) 383
- Evaluation of luminescence decay measurements probed on pure and doped Pt(IV) hexahalogeno complexes I. Exponential rise time and decay curves applying various statistical tests, I. Biertümpel and H.-H. Schmidtke 215 (1997) 271
- Factors affecting adiabaticity in bimolecular photoinduced electron transfer reaction between anthracene derivatives and organic donors, X. Allonas and P. Jacques 215 (1997) 371
- Matrix-isolated oxygen: line-shapes and transition probabilities of the $\text{b}^1\Sigma_g^+ \rightarrow \text{X}^3\Sigma_g^-$, $\text{b}^1\Sigma_g^+ \rightarrow \text{a}^1\Delta_g$ and $\text{a}^1\Delta_g \rightarrow \text{X}^3\Sigma_g^-$ transitions, G. Tyczkowski, U. Schurath, M. Bodenbinder and H. Willner 215 (1997) 379
- Sol-gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion, S.G. Kulikov, A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot 216 (1997) 147
- Sol-gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis, S.M. Arabei, S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup 216 (1997) 163
- Photophysics of *trans*-stilbene analogues: indolo[3,2-*b*]indole and its heterosubstituted sulfur and selenium derivatives, S. Dobrin, P. Kaszynski, S. Ikeda and J. Waluk 216 (1997) 179
- Analysis of the $\text{D}'2_g - \text{A}'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry, D. Cerny, R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota 216 (1997) 207
- Crystal structure and photoluminescence of single crystals of fullerene-9,9'-*trans*-bis(telluraxanthenyl) molecular complex: $\text{C}_{26}\text{H}_{18}\text{Te}_2 \cdot \text{C}_{60} \cdot \text{CS}_2$, V.V. Kveder, E.A. Steinman, B.Zh. Narymbetov, S.S. Khasanov, L.P. Rozenberg, R.P. Shibaeva, A.V. Bazhenov, A.V. Gorbunov, M.Yu. Maksimuk, D.V. Konarev, R.N. Lyubovskaya and Yu.A. Ossipyan 216 (1997) 407
- Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy, J. Widengren, J. Dapprich and R. Rigler 216 (1997) 417
- Vibron-mediated electronic relaxation in crystalline chlorine, D. Logan, C.A. Wight and V.A. Apkarian 217 (1997) 99
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmansröben 218 (1997) 175
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2 , E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309
- Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push-pull diphenyl-polyenes: evidence for 'loose' complex and 'bimer' species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73

- Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Milli   219 (1997) 265
- Fluorescence excitation spectroscopy of some haloethenes, $\text{CF}_2=\text{CXY}$ ($\text{XY} \equiv \text{FCl}, \text{Cl}_2, \text{FH}$), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H.   gren 220 (1997) 79
- Reaction dynamics of the $\text{Ca}(^1\text{D}_2, ^3\text{P}_J) + \text{CH}_3\text{I} \rightarrow \text{CaI}^* + \text{CH}_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. Gonz  lez Ure  a 220 (1997) 337
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355

Photoelectron and Auger spectroscopy

- Vibrational structure of the BrCN^+ ion from high resolution photoelectron spectroscopy, J.H.D. Eland, P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson 212 (1996) 457
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Charge-transfer states and the band gap in crystalline fullerene, A. Eilmes, R.W. Munn, B. Pac and P. Petelenz 214 (1997) 341
- Threshold photoelectron spectroscopy of SF_6 , A.J. Yench, D.B. Thompson, A.J. Cormack, D.R. Cooper, M. Zubek, P. Bolognesi and G.C. King 216 (1997) 227
- A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 , D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
- The He(I) , threshold photoelectron and constant ion state spectroscopy of vinylchloride ($\text{C}_2\text{H}_3\text{Cl}$), R. Locht, B. Leyh, K. Hottmann and H. Baumg  rtel 220 (1997) 217
- Extended Fenske–Hall LCAO MO calculations of core-level shifts in solid P compounds, R. Franke, T. Chass  , J. Reinhold, P. Streubel and R. Szargan 220 (1997) 299

X-ray spectroscopy

- Experimental and theoretical study of the C_{1s} shakeup spectra from biphenyl and p-terphenyl, C. Enkvist, S. Lunell and S. Svensson 214 (1997) 123
- Spectroscopic properties of chlorophylls and their derivatives. Influence of molecular structure on the electronic state, Y. Nonomura, S. Igarashi, N. Yoshioka and H. Inoue 220 (1997) 155

Electron impact spectroscopy

- Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine, Y. Zheng, C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen 212 (1996) 269
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- The formation and dissociation of the dinitrogen pentoxide dication, C.S.S. O'Connor, N.C. Jones and S.D. Price 214 (1997) 131

- Polarization propagator study of electronic excitation in key heterocyclic molecules I. Pyrrole, A.B. Trofimov and J. Schirmer 214 (1997) 153
- Imaging of the HOMO electron density in $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ by electron momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations, J. Rolke, Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy 215 (1997) 191
- Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3 : absolute oscillator strengths and dipole-induced breakdown pathways, J.W. Au, G. Cooper and C.E. Brion 215 (1997) 397
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- VUV optical-absorption and electron-energy-loss spectroscopy of formamide, J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel 220 (1997) 191
- Laser methods*
- Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye, M.A. Drobizhev, M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky 211 (1996) 455
- Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique, F.F. Brazgun, V.A. Nadochenko, I.V. Rubtsov and L.V. Lukin 211 (1996) 469
- Comment on “energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm”, S.W. North, T.J. Sears, G.E. Hall and T. Suzuki 211 (1996) 515
- Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Reported blue upconversion from U^{4+} doped into Cs_2ZrCl_6 single crystals under green laser excitation, P.A. Tanner, J. Dexpert-Ghys, Z.W. Pei and J. Lin 215 (1997) 125
- The van der Waals vibrational frequencies of the aniline–carbon monoxide complex in its S_1 state, J.-G. Jäckel, R. Schmid, H. Jones, T. Nakanaga and H. Takeo 215 (1997) 291
- Analysis of the $\text{D}'2_g - \text{A}'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry, D. Cerny, R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota 216 (1997) 207
- Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion, H. Hulsman 217 (1997) 107
- A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables, Y. Watanabe, H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura 217 (1997) 317
- A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces, W. Jakubetz and B.L. Lan 217 (1997) 375
- Learning control of quantum-mechanical systems by laboratory identification of effective input–output maps, M.Q. Phan and H. Rabitz 217 (1997) 389

- Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $\text{Cs}_2\text{NaCeCl}_6$, M. Chua and P.A. Tanner 218 (1997) 83
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- Intermolecular vibrations of the van der Waals complex $p\text{-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$, Y. Hu, W. Lu and S. Yang 218 (1997) 325
- Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221

Picosecond spectroscopy

- The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria, V.I. Novoderezhkin and A.P. Razjivin 211 (1996) 203
- Higher excited-state triplet–singlet intersystem crossing of some organic dyes, S. Reindl and A. Penzkofer 211 (1996) 431
- Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution, E.R. Middelhoeck, H. Zhang, J.W. Verhoeven and M. Glasbeek 211 (1996) 489
- Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy, L. Ujj, F. Jäger, A. Popp and G.H. Atkinson 212 (1996) 421
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière 214 (1997) 409
- Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Non-linear optical spectroscopy

- Higher excited-state triplet–singlet intersystem crossing of some organic dyes, S. Reindl and A. Penzkofer 211 (1996) 431
- Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques, P.C. Ray, N. Munichandiah and P.K. Das 211 (1996) 499
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière 214 (1997) 409
- Femtosecond dynamics of excited states in sexithiophene thin films, G. Klein, C. Jundt, B. Sipp, A.A. Villaeys, A. Boeglin, A. Yassar, G. Horowitz and F. Garnier 215 (1997) 131
- Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation, J.M. Luis, J. Martí, M. Duran and J.L. Andrés 217 (1997) 29
- Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Synchrotron spectroscopies

- Intracuster ion–molecule reactions induced by the synchrotron radiation in allyl bromide–ammonia clusters, C. Dedonder-Lardeux, C. Jouvét, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard 212 (1996) 371
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- A quasi-atomic treatment of chemical and structural effects on K-shell excitations in hexagonal and cubic BN crystals, R. Franke, S. Bender, J. Hormes, A.A. Pavlychev and N.G. Fominykh 216 (1997) 243
- Clusters containing BF_3 , $\text{O}(\text{CH}_3)_2$ and aromatic compounds: An electron impact and photoionization study, C.G. Eisenhardt, S. Ring, H.-W. Jochims and H. Baumgärtel 216 (1997) 427
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 , D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
- Fluorescence excitation spectroscopy of some haloethenes, $\text{CF}_2=\text{CXY}$ ($\text{XY} \equiv \text{FCl}, \text{Cl}_2, \text{FH}$), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
- VUV optical-absorption and electron-energy-loss spectroscopy of formamide, J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel 220 (1997) 191
- The photoabsorption spectrum of vinylchloride ($\text{C}_2\text{H}_3\text{Cl}$) in the 8–12 eV range, R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 207
- The He(I), threshold photoelectron and constant ion state spectroscopy of vinylchloride ($\text{C}_2\text{H}_3\text{Cl}$), R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 217

Coherent optical spectroscopy

- Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects, S.J. Zilker and D. Haarer 220 (1997) 167

Optical pumping

- Photoacoustic spectra of BaFBr:Eu^{2+} phosphors, Y. Zhang 219 (1997) 353

Multiple resonance spectroscopy

- Infrared spectroscopy of aniline–X ($\text{X} = \text{N}_2, \text{CH}_4, \text{CHF}_3, \text{CO}$) clusters and their corresponding cluster cations in the NH_2 -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

Optoacoustic spectroscopy

- Multiple absorption and relaxation processes in $\text{SF}_6\text{--CH}_4$ mixtures: an experimental study, J. Jovanovic-Kurepa, D.D. Markusev and M. Terzic 211 (1996) 347
- Spectroscopic investigation of ground state pyrrole ($^{12}\text{C}_4\text{H}_5\text{N}$): the N–H stretch, A. Mellouki, R. Georges, M. Herman, D.L. Snavely and S. Leytner 220 (1997) 311

Atomic and molecular beam techniques

- Intracuster ion–molecule reactions induced by the synchrotron radiation in allyl bromide–ammonia clusters, C. Dedonder-Lardeux, C. Jouvet, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard 212 (1996) 371
- Single electron capture in low-energy $\text{Kr}^+ - \text{He}$ collisions, H. Martínez and J.M. Hernandez 215 (1997) 285
- Fine-structure dependence of the $\text{Ar}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer process, E.J.D. Vredenbregt, W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 259
- $\text{Ar}^*(^3\text{P}_2)/\text{Kr}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer collisions: final state rotational alignment, E.J.D. Vredenbregt, W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 273
- The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione, A.A. Ruth, F.J. O’Keeffe, R.P. Brint and M.W.D. Mansfield 217 (1997) 83
- Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion, H. Hulsman 217 (1997) 107
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Intermolecular vibrations of the van der Waals complex $\text{p-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$, Y. Hu, W. Lu and S. Yang 218 (1997) 325
- Fluorescence excitation spectroscopy of some haloethenes, $\text{CF}_2 = \text{CXY}$ ($\text{XY} \equiv \text{FCl}, \text{Cl}_2, \text{FH}$), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
- Reaction dynamics of the $\text{Ca}(^1\text{D}_2, ^3\text{P}_J) + \text{CH}_3\text{I} \rightarrow \text{CaI}^* + \text{CH}_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña 220 (1997) 337

Time-resolved experiments

- Experimental and theoretical study of the recombination reaction of FC(O)O radicals, A.E. Croce, C.J. Cobos and E. Castellano 211 (1996) 215
- Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans–cis photoisomerisation, Yu.V. Il'ichev, W. Kühnle and K.A. Zachariasse 211 (1996) 441
- Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique, F.F. Brazgun, V.A. Nadtochenko, I.V. Rubtsov and L.V. Lukin 211 (1996) 469
- Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution, E.R. Middelhoek, H. Zhang, J.W. Verhoeven and M. Glasbeek 211 (1996) 489
- The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines, J.M. Warman, P.G. Schouten, G.H. Gelinck and M.P. de Haas 212 (1996) 183
- Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence, V.F. Tarasov, H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob 212 (1996) 353
- Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy, L. Ujj, F. Jäger, A. Popp and G.H. Atkinson 212 (1996) 421

- Time-resolved electroluminescence from single and bilayer LEDs based upon substituted poly-arylenevinylenes, Y.-H. Tak, H. Vestweber, H. Bässler, A. Bleyer, R. Stockmann and H.-H. Hörhold 212 (1996) 471
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution, S.A. Bagnich 214 (1997) 351
- The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF_3X^+ ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) ions, H. Biehl, K.J. Boyle, D.M. Smith and R.P. Tuckett 214 (1997) 357
- Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière 214 (1997) 409
- Calculation of triplet–singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs, K.M. Salikhov, J. Schlüpmann, M. Plato and K. Möbius 215 (1997) 23
- Peculiarities of the enthalpy relaxation of a glassy crystal, O. Delcourt, M. Descamps, J. Even, M. Bertault and J.F. Willart 215 (1997) 51
- Evaluation of luminescence decay measurements probed on pure and doped Pt(IV) hexahalogeno complexes I. Exponential rise time and decay curves applying various statistical tests, I. Biertümpel and H.-H. Schmidtke 215 (1997) 271
- A study of the hydration of aluminate minerals based on the measurements of the mean and the variance of the proton magnetic resonance relaxation rate, A.B. Kudryavtsev, T.V. Kouznetsova, W. Linert and G. Hunter 215 (1997) 419
- Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA, V.V. Eremenko, V.A. Karachevtsev and V.V. Slavin 216 (1997) 1
- Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing, B.D. Fainberg and B. Zolotov 216 (1997) 7
- Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis–trans photoisomerization dynamics, G. Ponterini 216 (1997) 193
- On the determination of $D_0^0(\text{CaBr})$ from translational energy threshold measurements, M. Garay Salazar, J.M. Orea and A. González Ureña 216 (1997) 365
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmansröben 218 (1997) 175
- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331
- Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for 'loose' complex and 'bimimer' species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73
- Non-exponential decays of the S_1 vibronic levels of acetaldehyde, S.-H. Lee and I.-C. Chen 220 (1997) 175
- Effects of CCl_4 on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions, M.F. Ferreira Marques, H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre 220 (1997) 233

- Ionization and fragmentation of OCS and CS₂ after photoexcitation around the sulfur 2p edge, U. Ankerhold, B. Esser and F. von Busch 220 (1997) 393

Mass spectrometry

- Translational spectroscopy of H⁺ produced by collision induced dissociation of H₃⁺ on He, H. Martinez and A. Amaya-Tapia 211 (1996) 299
- Comment on "energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm", S.W. North, T.J. Sears, G.E. Hall and T. Suzuki 211 (1996) 515
- Intracuster ion–molecule reactions induced by the synchrotron radiation in allyl bromide–ammonia clusters, C. Dedonder-Lardeux, C. Jouvet, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard 212 (1996) 371
- The formation and dissociation of the dinitrogen pentoxide dication, C.S.S. O'Connor, N.C. Jones and S.D. Price 214 (1997) 131
- Clusters containing BF₃, O(CH₃)₂ and aromatic compounds: An electron impact and photoionization study, C.G. Eisenhardt, S. Ring, H.-W. Jochims and H. Baumgärtel 216 (1997) 427
- Quantitative studies of the photoabsorption and photoionization of PCl₃ in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Intermolecular vibrations of the van der Waals complex p-C₆H₄FCH₃... Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325
- Nonradiative processes and infrared emission in matrix isolated ND, N. Caspary, B.E. Wurfel, A.M. Smith and V.E. Bondybey 220 (1997) 241

Radiolysis

- Time evolution of the rate constant for the tunneling reaction H₂ + D → H + HD in solid D₂–H₂ mixtures at very low temperature, T. Kumada, Y. Aratono and T. Miyazaki 212 (1996) 177

Mössbauer spectroscopy

- Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy, I. Chang, H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak 212 (1996) 221
- A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability, F. Varret, J. Linares and K. Boukheddaden 212 (1996) 487

X-ray, electron and neutron diffraction

- Orientational correlations in liquid carbon tetrabromide: a neutron diffraction and RMC study, I. Bakó, J.C. Dore and D.W. Huxley 216 (1997) 119
- Crystal structure and photoluminescence of single crystals of fullerene–9,9'-*trans*-bis(teluraxanthenyl) molecular complex: C₂₆H₁₈Te₂ · C₆₀ · CS₂, V.V. Kveder, E.A. Steinman, B.Zh. Narymbetov, S.S. Khasanov, L.P. Rozenberg, R.P. Shibaeva, A.V. Bazhenov, A.V. Gorbunov, M.Yu. Maksimuk, D.V. Konarev, R.N. Lyubovskaya and Yu.A. Ossipyan 216 (1997) 407

Neutron scattering

- Tunnelling of the one-dimensional rotor NH₃D⁺ in the NH₄ClO₄ and NH₄PF₆ lattices, H.G. Büttner, G.J. Kearley and B. Frick 214 (1997) 425
- The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid, M.R. Johnson, M. Neumann, B. Nicolai, P. Smith and G.J. Kearley 215 (1997) 343

- Inelastic neutron scattering studies of polyanilines and partially deuterated analogues, F. Fillaux, N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colombar, A. Gruger, A. Régis and L.T. Yu 216 (1997) 281
- Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine, G.J. Kearley, J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez 216 (1997) 323
- Light scattering*
- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465
- Degree of aggregation of indocyanine green in aqueous solutions determined by Mie scattering, R. Weigand, F. Rotermund and A. Penzkofer 220 (1997) 373
- Field emission and field ionization*
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- Measurement of macroscopic variables*
- Solvent effects on sol–gel transition of alginate solutions by addition of cupric ions, H. Zheng, K. Jiang, Q. Zhang and J. Wang 211 (1996) 507
- Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na₂O, V.M. Syutkin and V.A. Tolkatchev 212 (1996) 149
- Electric permittivity in the one- and two-phase region of 1-nitropropane–hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483
- Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures, A. Baranowski, K. Jerie and J. Gliński 214 (1997) 143
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation, W. Lorenz, M. Handschuh and F. Bergmann 215 (1997) 139
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions, F. Bergmann, M. Handschuh and W. Lorenz 215 (1997) 157

Objects

Bulk systems

Gases

- Transport coefficients for NO⁺ ions in helium gas: a test of the NO⁺–He interaction potential, L.A. Viehland, A.S. Dickinson and R.G.A.R. MacLagan 211 (1996) 1
- Correlated electronic potential-energy surfaces for proton interactions with N₂, F.A. Gianturco, S. Kumar and F. Schneider 211 (1996) 33
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region, A.L. Jones, A.J. Blake, L. Torop and D.G. McCoy 211 (1996) 291

- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- Multiple absorption and relaxation processes in $\text{SF}_6\text{--CH}_4$ mixtures: an experimental study, J. Jovanovic-Kurepa, D.D. Markusev and M. Terzic 211 (1996) 347
- Absorption cross section measurements of water vapor in the wavelength region 120 to 188 nm, K. Yoshino, J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui 211 (1996) 387
- Fast-ion beam laser spectroscopy of $^{14}\text{N}_2^+$ and $^{15}\text{N}_2^+$: high-resolution study of the (1, 2) band of the $\text{B } ^2\Sigma_u^+ \text{--} \text{X } ^2\Sigma_g^+$ system, K. Boudjarane, A. Alikacem and M. Larzillière 211 (1996) 393
- Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine, Y. Zheng, C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen 212 (1996) 269
- Vibrational structure of the BrCN^+ ion from high resolution photoelectron spectroscopy, J.H.D. Eland, P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson 212 (1996) 457
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Interatomic potentials for XO^+ and B^3I states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- On the calculation of hydrogen NMR chemical shielding, D.B. Chesnut 214 (1997) 73
- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the $\text{FCO} + \text{H}_2 \rightarrow \text{HFCO} + \text{H}$ abstraction reaction, J.S. Francisco 214 (1997) 213
- The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF_3X^+ ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) ions, H. Biehl, K.J. Boyle, D.M. Smith and R.P. Tuckett 214 (1997) 357
- Vacuum-UV fluorescence spectroscopy of CF_3X ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) in the range 10–30 eV, H. Biehl, K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims 214 (1997) 367
- Drift velocity of ions in lighter gases in electric and magnetic fields, L. Ferrari and A. Carbognani 215 (1997) 37
- Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region, A. Fahr, P. Hassanzadeh, B. Laszlo and R.E. Huie 215 (1997) 59
- Interaction forces and energy transfer dynamics of $\text{LiH} (^1\Sigma^+)$ and helium atoms. I. The ab initio evaluation of the lowest potential energy surface, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper 215 (1997) 227
- Interaction forces and energy transfer dynamics of $\text{LiH} (^1\Sigma^+)$ and helium atoms. II. Rotationally inelastic collisions and excitation efficiency, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi and M. Sironi 215 (1997) 239
- Cotton–Mouton effect and shielding polarizabilities of ethylene: an MCSCF study, S. Coriani, A. Rizzo, K. Ruud and T. Helgaker 216 (1997) 53
- Analysis of the $\text{D}'2_g\text{--}\text{A}'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry, D. Cerny, R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota 216 (1997) 207
- Effect of strong excitation of the CO_2 asymmetric mode on transport properties, A. Chikhaoui and E.V. Kustova 216 (1997) 297
- Isotope effects on the rate constants for the processes $\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O}_2$ and $\text{O}_2 + \text{O} + \text{Ar} \rightarrow \text{O}_3 + \text{Ar}$. On a modified ground-state potential energy surface for ozone, A. Gross and G.D. Billing 217 (1997) 1

- Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion, H. Hulsman 217 (1997) 107
- VUV optical-absorption and electron-energy-loss spectroscopy of formamide, J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel 220 (1997) 191
- The photoabsorption spectrum of vinylchloride (C_2H_3Cl) in the 8–12 eV range, R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 207
- The He(I), threshold photoelectron and constant ion state spectroscopy of vinylchloride (C_2H_3Cl), R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 217

Supersonic beams

- Ab initio calculations of the rovibrational states of He_2N^{2+} , J.M. Hughes and E.I. von Nagy-Felsobuki 211 (1996) 135
- Potential energy curve of the $X0^+(^1\Sigma^+)$ ground state of HgAr determined from $A0^+(^3\Pi) \rightarrow X0^+$ and $B1(^3\Sigma^+) \rightarrow X0^+$ fluorescence spectra, J. Koperski 211 (1996) 191
- Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam, A. Obrebski, T. Kaps and U. Cerny 212 (1996) 311
- The van der Waals vibrational frequencies of the aniline–carbon monoxide complex in its S_1 state, J.-G. Jäckel, R. Schmid, H. Jones, T. Nakanaga and H. Takeo 215 (1997) 291
- The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione, A.A. Ruth, F.J. O'Keeffe, R.P. Brint and M.W.D. Mansfield 217 (1997) 83
- A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Non-exponential decays of the S_1 vibronic levels of acetaldehyde, S.-H. Lee and I.-C. Chen 220 (1997) 175
- Spectroscopic investigation of ground state pyrrole ($^{12}C_4H_5N$): the N–H stretch, A. Mellouki, R. Georges, M. Herman, D.L. Snively and S. Leytner 220 (1997) 311

Liquids neat

- Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans–cis photoisomerisation, Yu.V. Il'ichev, W. Kühnle and K.A. Zachariasse 211 (1996) 441
- An analytical study of the Berezhkovskii–Pollak–Zitserman theory of rate processes in the critical region. II. The critical coupling plane, S. Singh and G.W. Robinson 212 (1996) 125
- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465
- Orientational correlations in liquid carbon tetrabromide: a neutron diffraction and RMC study, I. Bakó, J.C. Dore and D.W. Huxley 216 (1997) 119
- Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235

Liquid mixtures and solutions

- Solvent reorganization energy of electron transfer in weakly polar solvents, D.V. Matyushov 211 (1996) 47
- A QM/MM simulation method applied to the solution of Li^+ in liquid ammonia, T. Kerdcharoen, K.R. Liedl and B.M. Rode 211 (1996) 313

- Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution, E.R. Middelhoek, H. Zhang, J.W. Verhoeven and M. Glasbeek 211 (1996) 489
- Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques, P.C. Ray, N. Munichandiah and P.K. Das 211 (1996) 499
- Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations, H. Sumi 212 (1996) 9
- Recovering boundaries for partly diffusion-controlled reaction kinetics, N.J.B. Green, R.D. Spencer-Smith and A.G. Rickerby 212 (1996) 99
- An analytical study of the Berezhkovskii–Pollak–Zitserman theory of rate processes in the critical region. II. The critical coupling plane, S. Singh and G.W. Robinson 212 (1996) 125
- Temperature dependence of the density of an ionic micellar system near the critical point, A. Compostizo, C. Martín, R.G. Rubio and A. Crespo Colin 212 (1996) 301
- Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence, V.F. Tarasov, H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob 212 (1996) 353
- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejcki, G. Waliszewska and H. Abramczyk 213 (1996) 341
- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Electric permittivity in the one- and two-phase region of 1-nitropropane–hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483
- Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures, A. Baranowski, K. Jerie and J. Gliński 214 (1997) 143
- On the degrees of circularity for various kinds of polarized light in a nonpolar liquid mixture, D.J. Lee and K.-R. Kim 214 (1997) 183
- Factors affecting adiabaticity in bimolecular photoinduced electron transfer reaction between anthracene derivatives and organic donors, X. Allonas and P. Jacques 215 (1997) 371
- Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing, B.D. Fainberg and B. Zolotov 216 (1997) 7
- Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis–trans photoisomerization dynamics, G. Ponterini 216 (1997) 193
- Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines, W. Werncke, M. Pfeiffer, T. Johr, A. Lau, W. Grahm, H.-H. Johannes and L. Dähne 216 (1997) 337
- Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose, B. Leroux, H. Bizot, J.W. Brady and V. Tran 216 (1997) 349

- Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy, J. Widengren, J. Dapprich and R. Rigler 216 (1997) 417
- Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases, M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer 217 (1997) 259
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
- Statistical mechanical treatment of reactive solvent extraction, M. Lukhezo, L.J. Dunne, B.G. Reuben and M.S. Verrall 220 (1997) 53
- Effects of CCl₄ on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions, M.F. Ferreira Marques, H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre 220 (1997) 233
- Structure and dynamics at the surface of a concentrated aqueous solution of CsF, J. Dietter and H. Morgner 220 (1997) 261
- Forward and reverse excitation energy transport in concentrated two-component systems, P. Bojarski and L. Kułak 220 (1997) 323

Crystals

- Al,Si ordering in chabazites: A Monte Carlo study, M.C. Gordillo and C.P. Herrero 211 (1996) 81
- Stochastic wave packet vs. direct density matrix solution of Liouville–von Neumann equations for photodesorption problems, P. Saalfrank 211 (1996) 265
- An ab initio perturbed ion study of structural properties of TiO₂, SnO₂ and GeO₂ rutile lattices, A.C. Camargo, J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés 212 (1996) 381
- A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability, F. Varret, J. Linares and K. Boukheddaden 212 (1996) 487
- Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er³⁺ in YVO₄, J.A. Capobianco, P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli 214 (1997) 329
- Peculiarities of the enthalpy relaxation of a glassy crystal, O. Delcourt, M. Descamps, J. Even, M. Bertault and J.F. Willart 215 (1997) 51
- Rotation/precession of NH₃ groups in Hofmann clathrates, M. Neumann and G.J. Kearley 215 (1997) 253
- Charge-transfer excitons in the dielectric theory of molecular crystals, R.W. Munn 215 (1997) 301
- The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid, M.R. Johnson, M. Neumann, B. Nicolai, P. Smith and G.J. Kearley 215 (1997) 343
- A quasi-atomic treatment of chemical and structural effects on K-shell excitations in hexagonal and cubic BN crystals, R. Franke, S. Bender, J. Hormes, A.A. Pavlychev and N.G. Fominykh 216 (1997) 243
- Crystal structure and photoluminescence of single crystals of fullerene–9,9'-*trans*-bis(telluraxanthenyl) molecular complex: C₂₆H₁₈Te₂ · C₆₀ · CS₂, V.V. Kveder, E.A. Steinman, B.Zh. Narymbetov, S.S. Khasanov, L.P. Rozenberg, R.P. Shibaeva, A.V. Bazhenov, A.V. Gorbunov, M.Yu. Maksimuk, D.V. Konarev, R.N. Lyubovskaya and Yu.A. Ossipyan 216 (1997) 407
- Extended Fenske–Hall LCAO MO calculations of core-level shifts in solid P compounds, R. Franke, T. Chassé, J. Reinhold, P. Streubel and R. Szargan 220 (1997) 299

-neat

- Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR, N.A. Salih, O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen 212 (1996) 409
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Charge-transfer states and the band gap in crystalline fullerene, A. Eilmes, R.W. Munn, B. Pac and P. Petelenz 214 (1997) 341
- Vibron-mediated electronic relaxation in crystalline chlorine, D. Logan, C.A. Wight and V.A. Apkarian 217 (1997) 99
- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

-mixed

- Single molecule polarization spectroscopy: pentacene in p-terphenyl, F. Güttler, M. Croci, A. Renn and U.P. Wild 211 (1996) 421
- Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy, I. Chang, H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak 212 (1996) 221
- Reported blue upconversion from U^{4+} doped into Cs_2ZrCl_6 single crystals under green laser excitation, P.A. Tanner, J. Dexpert-Ghys, Z.W. Pei and J. Lin 215 (1997) 125
- Matrix-isolated oxygen: line-shapes and transition probabilities of the $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$, $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ and $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transitions, G. Tyczkowski, U. Schurath, M. Bodenbinder and H. Willner 215 (1997) 379
- Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA, V.V. Eremenko, V.A. Karachevtsev and V.V. Slavin 216 (1997) 1
- Structure and selective visible photodissociation of the $O_3:Br_2$ and $O_3:BrCl$ complexes: an infrared matrix isolation and ab initio study, M. Bahou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 216 (1997) 105
- The tunneling frequencies of the isotopic forms of methane in rare-gas solids, D. Smith 220 (1997) 279

Glasses

- Kohlrausch relaxation in electronic and molecular glasses, J.C. Phillips 212 (1996) 41
- Comments on the mode coupling theory for structural relaxation, W. Götze and L. Sjögren 212 (1996) 47
- Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na_2O , V.M. Syutkin and V.A. Tolkachev 212 (1996) 149
- Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution, S.A. Bagnich 214 (1997) 351
- Peculiarities of the enthalpy relaxation of a glassy crystal, O. Delcourt, M. Descamps, J. Even, M. Bertault and J.F. Willart 215 (1997) 51
- Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives, V.L. Vyazovkin and V.A. Tolkachev 216 (1997) 135
- Sol-gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion, S.G. Kulikov, A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot 216 (1997) 147
- Sol-gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis, S.M. Arabei, S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup 216 (1997) 163

- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects, S.J. Zilker and D. Haarer 220 (1997) 167
- Liquid crystals*
- Order parameters and carbon shielding tensors of bis-MSB from ^{13}C NMR measurements in a nematic liquid crystal, R. Tarroni and C. Zannoni 211 (1996) 337
- The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines, J.M. Warman, P.G. Schouten, G.H. Gelinck and M.P. de Haas 212 (1996) 183
- A new potential for the description of intermolecular interactions for rigid biaxial molecules, V.V. Ginzburg, M.A. Glaser and N.A. Clark 214 (1997) 253
- Polymers*
- Irreversible random transition theory as applied to rate processes in condensed media: Transient effects of constrained configuration rearrangements in complex systems, Yu.A. Berlin 212 (1996) 29
- Time-resolved electroluminescence from single and bilayer LEDs based upon substituted poly-arylenevinylenes, Y.-H. Tak, H. Vestweber, H. Bässler, A. Bleyer, R. Stockmann and H.-H. Hörhold 212 (1996) 471
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- Inelastic neutron scattering studies of polyanilines and partially deuterated analogues, F. Fillaux, N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colombari, A. Gruger, A. Régis and L.T. Yu 216 (1997) 281
- Dynamical resonance and tunneling in a driven system with periodic potential, E.M. Zanardi and J.M. Gomez Llorente 217 (1997) 221
- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331
- Semiconductors*
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation, W. Lorenz, M. Handschuh and F. Bergmann 215 (1997) 139
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions, F. Bergmann, M. Handschuh and W. Lorenz 215 (1997) 157
- Ultracold atoms in modulated standing light waves, K. Drese and M. Holthaus 217 (1997) 201
- Dynamical resonance and tunneling in a driven system with periodic potential, E.M. Zanardi and J.M. Gomez Llorente 217 (1997) 221
- Photoacoustic spectra of BaFBr:Eu^{2+} phosphors, Y. Zhang 219 (1997) 353
- Metals and alloys*
- Vibronic theory of electric hysteresis in "bistable" mixed-valence molecular salts, K. Boukheddaden and F. Varret 216 (1997) 373

Thin films

- The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film, J.M. Muller, D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen 211 (1996) 413
- Time-resolved electroluminescence from single and bilayer LEDs based upon substituted poly-arylenevinylenes, Y.-H. Tak, H. Vestweber, H. Bässler, A. Bleyer, R. Stockmann and H.-H. Hörhold 212 (1996) 471
- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Femtosecond dynamics of excited states in sexithiophene thin films, G. Klein, C. Jundt, B. Sipp, A.A. Villaeys, A. Boeglin, A. Yassar, G. Horowitz and F. Garnier 215 (1997) 131

Surfaces

- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- Structures and potential energy surface of Faujasitic zeolite/water, J. Limtrakul, P. Treesukol, C. Ebner, R. Sansone and M. Probst 215 (1997) 77
- Disordered surfaces: a smoothed He–target scattering potential for metal atoms adsorbed on metal surfaces, G. Petrella, L. Cassidei and F. Ciriaco 216 (1997) 391
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Theoretical study on adsorption and proton exchange reaction of H₂O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257
- Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy, J. Cortés and E. Valencia 219 (1997) 235
- Quantum effects in adiabatic electrochemical electron-transfer reactions, M.T.M. Koper, J.-H. Mohr and W. Schmickler 220 (1997) 95
- Scattering of large argon clusters from a Pt(111) surface with low collision velocities, M. Svanberg, N. Marković and J.B.C. Pettersson 220 (1997) 137

Low-dimensional materials

- Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye, M.A. Drobizhev, M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky 211 (1996) 455

Dielectrics

- Electric permittivity in the one- and two-phase region of 1-nitropropane–hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483
- Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium–water clusters, J.C. Contador, M.A. Aguilar and F.J.O. del Valle 214 (1997) 113
- Charge-transfer excitons in the dielectric theory of molecular crystals, R.W. Munn 215 (1997) 301
- Calculation of the solvent reorganization free energy in the dielectric cavity model, E.L. Mertz, E.D. German and A. M. Kuznetsov 215 (1997) 355

Plasmas

- Monte Carlo simulation studies on the validity of the Gram–Charlier calculations of velocity distributions of Na⁺ swarm in neon gas, P.P. Ong and M.-M. Li 211 (1996) 115

- Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulas 218 (1997) 57

Biological systems

- Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives, A. Broo and A. Holmén 211 (1996) 147
- The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria, V.I. Novoderezhkin and A.P. Razjivin 211 (1996) 203
- Molecular dynamics simulations of cis–trans isomerization for a proline-containing tripeptide in solution, S.Z. Wan, C.X. Wang, Y.W. Xu and Y.Y. Shi 211 (1996) 227
- Solvent effects on sol–gel transition of alginate solutions by addition of cupric ions, H. Zheng, K. Jiang, Q. Zhang and J. Wang 211 (1996) 507
- Dynamic effects in non-adiabatic charge transfer, E. Gudowska-Nowak 212 (1996) 115
- Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy, I. Chang, H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak 212 (1996) 221
- Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model, C. Scharnagl and S.F. Fischer 212 (1996) 231
- Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy, L. Ujj, F. Jäger, A. Popp and G.H. Atkinson 212 (1996) 421
- Water residence times around copper plastocyanin: a molecular dynamics simulation approach, C. Rocchi, A.R. Bizzarri and S. Cannistraro 214 (1997) 261
- Double exchange in distorted trimeric mixed-valence clusters, M.I. Belinsky 215 (1997) 7
- Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose, B. Leroux, H. Bizot, J.W. Brady and V. Tran 216 (1997) 349
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
- Phenomenological model for reaction kinetics coupled to a relaxing environment, Y.A. Berlin, A.L. Burin and S.F. Fischer 220 (1997) 25

Microscopic systems

Atoms

- Time evolution of the rate constant for the tunneling reaction $H_2 + D \rightarrow H + HD$ in solid D_2 – H_2 mixtures at very low temperature, T. Kumada, Y. Aratono and T. Miyazaki 212 (1996) 177
- The d -dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals and alternative Sturmian basis sets, V. Aquilanti, S. Cavalli and C. Coletti 214 (1997) 1
- Application of the pairwise energy model to various isotopic variations of the $H + H_2$ reaction, J.-B. Song and E.A. Gislason 214 (1997) 23
- The formalism and matrix elements of a complete potential-harmonic scheme for directly solving the Schrödinger equation of the helium atom, Y.-X. Wang and C.-H. Deng 214 (1997) 33
- Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations, J.W. Boughton, S. Kristyan and M.C. Lin 214 (1997) 219

- Calculation of ground- and excited-state potential energy curves for the Hg_2 molecule in a pseudopotential approach, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 214 (1997) 277
- A quantal entropy signature for the dynamics of pure states: Studies on some model problems, P. Sarkar, S. Adhikari and S.P. Bhattacharyya 215 (1997) 309
- Fine-structure dependence of the $\text{Ar}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer process, E.J.D. Vredenbregt, W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 259
- $\text{Ar}^*(^3\text{P}_2)/\text{Kr}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer collisions: final state rotational alignment, E.J.D. Vredenbregt, W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 273
- Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree–Fock method, F.E. Jorge, E.V.R. de Castro and A.B.F. da Silva 216 (1997) 317
- Spin–orbit interaction in heavy group 13 atoms and TlAr , T. Leininger, A. Berning, A. Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad 217 (1997) 19
- Theoretical study of multiple high-order harmonic generation by intense ultrashort pulsed laser fields: A new generalized pseudospectral time-dependent method, X.-M. Tong and S.-I. Chu 217 (1997) 119
- The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
- Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279
- Highly correlated QDPT-CI calculations of valence and core photoelectron spectra of Ne, G. Fronzoni and P. Decleva 220 (1997) 15
- A three-body calculation for collision-induced dissociation, K. Sakai 220 (1997) 115
- Classification of Cm I energy levels using PCA–BPN and PCA–NLM, X. Cao, H. Liu and N. Chen 220 (1997) 289
- Ionization and fragmentation of OCS and CS_2 after photoexcitation around the sulfur 2p edge, U. Ankerhold, B. Esser and F. von Busch 220 (1997) 393
- Molecules (neutral and ionic)*
- Magnetic field dependent yield of geminate radical pair recombination in micelles. Effect of intraradical spin lattice relaxation, J.S. Jørgensen, J.B. Pedersen and A.I. Shushin 211 (1996) 235
- Translational spectroscopy of H^- produced by collision induced dissociation of H_3^+ on He, H. Martinez and A. Amaya-Tapia 211 (1996) 299
- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- Generalized oscillator strengths for SF_6 in the S 2p inner-shell region, Z. Felfli, I. Fomunung, D. Bessis and A.Z. Msezane 211 (1996) 325
- Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques, P.C. Ray, N. Munichandiah and P.K. Das 211 (1996) 499
- Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam, A. Obrebski, T. Kaps and U. Cerny 212 (1996) 311
- Ab initio study on the electronic structure of the $4^2\Sigma^+$ and $5^2\Sigma^+$ excited states of CO^+ , N. Honjou and E. Miyoshi 212 (1996) 363
- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123

- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- Photodissociation dynamics of $HN_3(DN_3) + h\nu \rightarrow H(D) + N_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- The anharmonic effect as originated from the asymmetry of a rotor. The case study of an asymmetric rotor coupled with a simple harmonic oscillator, G. Wu 214 (1997) 15
- On the calculation of hydrogen NMR chemical shielding, D.B. Chesnut 214 (1997) 73
- Ab initio calculations of electronic spectra of H_2S and H_2S_2 , M. Pericou-Cayere, M. Gelize and A. Dargelos 214 (1997) 81
- Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations, J.W. Boughton, S. Kristyan and M.C. Lin 214 (1997) 219
- Ab initio calculations of S_1 excited state vibrational spectra of benzene, naphthalene and anthracene, G.S. Jas and K. Kuczera 214 (1997) 229
- Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I, J. Zhang and M. Baumgarten 214 (1997) 291
- A classical approach to resonant low-energy electron scattering off molecules: application to the a_1 -shape resonance of CF_3Cl , L. Lehr, J. Manz and W.H. Miller 214 (1997) 301
- Rotational and vibrational excitation of the N_2^+ (B) state in a $He + N_2$ electron-beam plasma, A.E. Belikov 215 (1997) 97
- Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters, R.G. Schmidt, M.C. Böhm and J. Brickmann 215 (1997) 207
- Rotation/precession of NH_3 groups in Hofmann clathrates, M. Neumann and G.J. Kearley 215 (1997) 253
- The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory, A. Beghin and T. Stoecklin 215 (1997) 261
- A quantal entropy signature for the dynamics of pure states: Studies on some model problems, P. Sarkar, S. Adhikari and S.P. Bhattacharyya 215 (1997) 309
- Effect of strong excitation of the CO_2 asymmetric mode on transport properties, A. Chikhaoui and E.V. Kustova 216 (1997) 297
- On the determination of $D_0^0(CaBr)$ from translational energy threshold measurements, M. Garay Salazar, J.M. Orea and A. González Ureña 216 (1997) 365
- Dynamical simulation of the driven spin-boson system: The influence of interblip correlations, M. Winterstetter and U. Weiss 217 (1997) 155
- Photodissociation of Ar_2^+ in strong laser fields, P. Schwendner, F. Seyl and R. Schinke 217 (1997) 233
- Simultaneous control of selectivity and yield of molecular dissociation. Pulsed incoherent interference control, M. Shapiro, Z. Chen and P. Brumer 217 (1997) 325

- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Theoretical study on adsorption and proton exchange reaction of H₂O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257
- Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff 219 (1997) 119
- Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A. Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143
- Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
- A three-body calculation for collision-induced dissociation, K. Sakai 220 (1997) 115
- diatomic*
- The dissociation energies of FeF, FeCl, and FeBr and their positive ions, C.W. Bauschlicher Jr. 211 (1996) 163
- Rydberg basis set effects on ab initio second hyperpolarizabilities of H₂, C₆H₆ and CS₂ molecules, T. Hamada 211 (1996) 171
- An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region, A.L. Jones, A.J. Blake, L. Torop and D.G. McCoy 211 (1996) 291
- Photophysics and photochemistry of I₂ (D, D') in rare gas clusters, K.L. Randall and D.J. Donaldson 211 (1996) 377
- Fast-ion beam laser spectroscopy of ¹⁴N₂⁺ and ¹⁵N₂⁺: high-resolution study of the (1, 2) band of the B²Σ_u⁺-X²Σ_g⁺ system, K. Boudjarane, A. Alikacem and M. Larzillière 211 (1996) 393
- Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine, Y. Zheng, C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen 212 (1996) 269
- Ab initio study on the electronic structure of the 4²Σ⁺ and 5²Σ⁺ excited states of CO⁺, N. Honjou and E. Miyoshi 212 (1996) 363
- Optically pumped laser emission in K₂ involving rovibrational levels near the B¹Π_u state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- Interatomic potentials for X0⁺ and B³1 states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Influence of the molecular environment on the hyperfine interaction of ¹¹¹Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- Application of the pairwise energy model to various isotopic variations of the H + H₂ reaction, J.-B. Song and E.A. Gislason 214 (1997) 23

- The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH^- and $\text{OH}^- \cdot \text{H}_2\text{O}$, S.P.A. Sauer, V. Špirko, I. Paidarová and W.P. Kraemer 214 (1997) 91
- Calculation of ground- and excited-state potential energy curves for the Hg_2 molecule in a pseudopotential approach, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 214 (1997) 277
- Is HeH^- a stable system?, G.L. Bendazzoli, S. Evangelisti and F. Passarini 215 (1997) 217
- Matrix-isolated oxygen: line-shapes and transition probabilities of the $\text{b}^1\Sigma_g^+ \rightarrow \text{X}^3\Sigma_g^-$, $\text{b}^1\Sigma_g^+ \rightarrow \text{a}^1\Delta_g$ and $\text{a}^1\Delta_g \rightarrow \text{X}^3\Sigma_g^-$ transitions, G. Tyczkowski, U. Schurath, M. Bodenbinder and H. Willner 215 (1997) 379
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases, M. Pulfer, C.-H. Hu and D.P. Chong 216 (1997) 91
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules, C.-H. Hu and D.P. Chong 216 (1997) 99
- Analysis of the $\text{D}'2_g - \text{A}'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry, D. Cerny, R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota 216 (1997) 207
- Fine-structure dependence of the $\text{Ar}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer process, E.J.D. Vredenbregt, W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 259
- $\text{Ar}^*(^3\text{P}_2)/\text{Kr}^*(^3\text{P}_{0,2}) + \text{N}_2(\text{X})$ excitation transfer collisions: final state rotational alignment, E.J.D. Vredenbregt, W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 273
- Isotope effects on the rate constants for the processes $\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O}_2$ and $\text{O}_2 + \text{O} + \text{Ar} \rightarrow \text{O}_3 + \text{Ar}$. On a modified ground-state potential energy surface for ozone, A. Gross and G.D. Billing 217 (1997) 1
- Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury, P. Backhaus and B. Schmidt 217 (1997) 131
- Photodissociation of Ar_2^+ in strong laser fields, P. Schwendner, F. Seyl and R. Schinke 217 (1997) 233
- Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule, H. Dietz, A. Materny and V. Engel 217 (1997) 249
- Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association, M.V. Korolkov, J. Manz and G.K. Paramonov 217 (1997) 341
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Rovibrational dependence of the nuclear quadrupole coupling constants of HF , OH^- and NeH^+ , J. Vojtík and J. Fišer 218 (1997) 13
- Simulation of the $\text{SiH} (\text{A}^2\Delta \rightarrow \text{X}^2\Pi)$ emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2 , E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309
- Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G. Granucci and M. Persico 219 (1997) 21

- “Free” nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43
- The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
- small polyatomics*
- Transport coefficients for NO^+ ions in helium gas: a test of the NO^+ –He interaction potential, L.A. Viehland, A.S. Dickinson and R.G.A.R. MacLagan 211 (1996) 1
- Selective rovibrational energy transfer: A classical trajectory study of collisional energy redistribution in methyl radical, G.S. Peng and R.P. Parson 211 (1996) 17
- Rydberg basis set effects on ab initio second hyperpolarizabilities of H_2 , C_6H_6 and CS_2 molecules, T. Hamada 211 (1996) 171
- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- Multiple absorption and relaxation processes in SF_6 – CH_4 mixtures: an experimental study, J. Jovanovic-Kurepa, D.D. Markusev and M. Terzic 211 (1996) 347
- Absorption cross section measurements of water vapor in the wavelength region 120 to 188 nm, K. Yoshino, J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui 211 (1996) 387
- Comment on “energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm”, S.W. North, T.J. Sears, G.E. Hall and T. Suzuki 211 (1996) 515
- Interstellar silicon–nitrogen chemistry. I. The microwave and the infrared signatures of the HSiN , HNSi , HSiNH_2 , HNSiH_2 and HSiNH^+ species, O. Parisel, M. Hanus and Y. Ellinger 212 (1996) 331
- Vibrational structure of the BrCN^+ ion from high resolution photoelectron spectroscopy, J.H.D. Eland, P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson 212 (1996) 457
- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- The ArCIF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- Ab initio determination of quasi-diabatic states for multiple reaction pathways, P. Cattaneo and M. Persico 214 (1997) 49
- The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH^- and $\text{OH}^- \cdot \text{H}_2\text{O}$, S.P.A. Sauer, V. Špirko, I. Paidarová and W.P. Kraemer 214 (1997) 91
- An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen, V. Sreedhara Rao and A.K. Chandra 214 (1997) 103
- The formation and dissociation of the dinitrogen pentoxide dication, C.S.S. O'Connor, N.C. Jones and S.D. Price 214 (1997) 131
- Polarization propagator study of electronic excitation in key heterocyclic molecules I. Pyrrole, A.B. Trofimov and J. Schirmer 214 (1997) 153

- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the $\text{FCO} + \text{H}_2 \rightarrow \text{HFCO} + \text{H}$ abstraction reaction, J.S. Francisco 214 (1997) 213
- A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices, J. Kölm, A. Engdahl, O. Schrems and B. Nelander 214 (1997) 313
- The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF_3X^+ ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) ions, H. Biehl, K.J. Boyle, D.M. Smith and R.P. Tuckett 214 (1997) 357
- Vacuum-UV fluorescence spectroscopy of CF_3X ($\text{X} = \text{F}, \text{H}, \text{Cl}, \text{Br}$) in the range 10–30 eV, H. Biehl, K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims 214 (1997) 367
- Tunnelling of the one-dimensional rotor NH_3D^+ in the NH_4ClO_4 and NH_4PF_6 lattices, H.G. Büttner, G.J. Kearley and B. Frick 214 (1997) 425
- Dipole polarizability and hyperpolarizability of FCN, ClCN, BrCN and ICN, G. Maroulis and C. Pouchan 215 (1997) 67
- Theoretical study of the low-lying excited states of ABCO, DABCO and homologous cage amines, V. Galasso 215 (1997) 183
- Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra, A.M. Mebel and S.-H. Lin 215 (1997) 329
- Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3 : absolute oscillator strengths and dipole-induced breakdown pathways, J.W. Au, G. Cooper and C.E. Brion 215 (1997) 397
- Cotton–Mouton effect and shielding polarizabilities of ethylene: an MCSCF study, S. Coriani, A. Rizzo, K. Ruud and T. Helgaker 216 (1997) 53
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules, C.-H. Hu and D.P. Chong 216 (1997) 99
- Threshold photoelectron spectroscopy of SF_6 , A.J. Yench, D.B. Thompson, A.J. Cormack, D.R. Cooper, M. Zubek, P. Bolognesi and G.C. King 216 (1997) 227
- Infrared bands of mass-selected carbon chains C_n ($n = 8\text{--}12$) and C_n^- ($n = 5\text{--}10, 12$) in neon matrices, P. Freivogel, M. Grutter, D. Forney and J.P. Maier 216 (1997) 401
- Isotope effects on the rate constants for the processes $\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O}_2$ and $\text{O}_2 + \text{O} + \text{Ar} \rightarrow \text{O}_3 + \text{Ar}$. On a modified ground-state potential energy surface for ozone, A. Gross and G.D. Billing 217 (1997) 1
- Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation, J.M. Luis, J. Martí, M. Duran and J.L. Andrés 217 (1997) 29
- A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH, X. Chapuisat, C. Saint-Espès, C. Zuhrt and L. Zülicke 217 (1997) 43
- Raman bandshape analysis of oxocarbon ions in aqueous solutions, M.C.C. Ribeiro, L.F.C. de Oliveira and P.S. Santos 217 (1997) 71
- A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables, Y. Watanabe, H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura 217 (1997) 317
- A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces, W. Jakubetz and B.L. Lan 217 (1997) 375
- Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p, 2s; Cl 2p, 2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87

- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
- Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
- Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
- A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 , D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
- Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2 –ClO complexes, S. Aloisio and J.S. Francisco 219 (1997) 201
- Theoretical study of cyclic radicals NO_x ($x = 2–6$), Y. Li and S. Iwata 219 (1997) 209
- Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
- Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305
- Diatomics-in-molecules study of the ground and excited states of H_3^- , A.K. Belyaev and A.S. Tiukanov 220 (1997) 43
- Non-exponential decays of the S_1 vibronic levels of acetaldehyde, S.-H. Lee and I.-C. Chen 220 (1997) 175
- The photoabsorption spectrum of vinylchloride (C_2H_3Cl) in the 8–12 eV range, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 207
- The He(I), threshold photoelectron and constant ion state spectroscopy of vinylchloride (C_2H_3Cl), R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 217
- Reaction dynamics of the $Ca(^1D_2, ^3P_J) + CH_3I \rightarrow CaI^* + CH_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña 220 (1997) 337
- Ionization and fragmentation of OCS and CS_2 after photoexcitation around the sulfur 2p edge, U. Ankerhold, B. Esser and F. von Busch 220 (1997) 393
- aromatics*
- Solvent reorganization energy of electron transfer in weakly polar solvents, D.V. Matyushov 211 (1996) 47
- Spin-orbit effects in fullerenes, F.J. Adrian 211 (1996) 73
- Rydberg basis set effects on ab initio second hyperpolarizabilities of H_2 , C_6H_6 and CS_2 molecules, T. Hamada 211 (1996) 171
- The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film, J.M. Muller, D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen 211 (1996) 413
- Single molecule polarization spectroscopy: pentacene in p-terphenyl, F. Güttler, M. Croci, A. Renn and U.P. Wild 211 (1996) 421

- Higher excited-state triplet–singlet intersystem crossing of some organic dyes, S. Reindl and A. Penzkofer 211 (1996) 431
- The charge transfer state of excited bianthryl and a derivative: solvatochromism, emission CT spectra broadening in homogeneous solvents, H. Laguitton-Pasquier, R. Pansu, J.-P. Chauvet, A. Collet, J. Faure and R. Lapouyade 212 (1996) 437
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Experimental and theoretical study of the C_{1s} shakeup spectra from biphenyl and p-terphenyl, C. Enkvist, S. Lunell and S. Svensson 214 (1997) 123
- Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state, P. Karafiloglou 214 (1997) 171
- The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel 214 (1997) 191
- Ab initio calculations of S_1 excited state vibrational spectra of benzene, naphthalene and anthracene, G.S. Jas and K. Kuczera 214 (1997) 229
- Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution, S.A. Bagnich 214 (1997) 351
- Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière 214 (1997) 409
- Hybridizations of fullerenes: their relations with properties and applications in computation, X.P. Yu, Z.L. Cao and R.S. Han 215 (1997) 1
- Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing, B.D. Fainberg and B. Zolotov 216 (1997) 7
- Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn–Teller distortion in the excited electronic state on Raman intensities, H. Torii, M. Tasumi, I.M. Bell and R.J.H. Clark 216 (1997) 67
- Photophysics of *trans*-stilbene analogues: indolo[3,2-*b*]indole and its heterosubstituted sulfur and selenium derivatives, S. Dobrin, P. Kaszynski, S. Ikeda and J. Waluk 216 (1997) 179
- Symmetrised quantum-mechanical force-fields and INS spectra: s-triazine, trichloro-s-triazine and pyrazine, G.J. Kearley, J. Tomkinson, A. Navarro, J.J. López González and M. Fernández Gómez 216 (1997) 323
- Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy, J. Widengren, J. Dapprich and R. Rigler 216 (1997) 417
- The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione, A.A. Ruth, F.J. O'Keeffe, R.P. Brint and M.W.D. Mansfield 217 (1997) 83
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for ‘loose’ complex and ‘bimer’ species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73
- The relationship between the molecular structure of semiquinone radicals and their *g*-values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291
- other large*
- Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution, E.R. Middelhoek, H. Zhang, J.W. Verhoeven and M. Glasbeek 211 (1996) 489
- An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen, V. Sreedhara Rao and A.K. Chandra 214 (1997) 103
- Spectroscopy and photophysics of $C_{60}H_{18}$ and $C_{60}H_{36}$, R.V. Bensasson, T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt 215 (1997) 111
- Femtosecond dynamics of excited states in sexithiophene thin films, G. Klein, C. Jundt, B. Sipp, A.A. Villaeys, A. Boeglin, A. Yassar, G. Horowitz and F. Garnier 215 (1997) 131
- Imaging of the HOMO electron density in $Cr(CO)_6$, $Mo(CO)_6$ and $W(CO)_6$ by electron momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations, J. Rolke, Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy 215 (1997) 191
- Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines, W. Werncke, M. Pfeiffer, T. Johr, A. Lau, W. Grahn, H.-H. Johannes and L. Dähne 216 (1997) 337
- Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases, M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer 217 (1997) 259
- Reverse saturable absorption in palladium and zinc tetraphenyltetraabenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301
- Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
- Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341
- Strong-field approach to ultrafast pump–probe spectra: dye molecules in solution, D.H. Schirrmeister and V. May 220 (1997) 1
- The magnetic field influence on bridge-assisted electron transfer, E.G. Petrov, I.S. Tolokh, V.V. Gorbach and V. May 220 (1997) 249
- polymeric and biological*
- Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives, A. Broo and A. Holmén 211 (1996) 147
- A temperature-dependent effective potential explains CO binding to myoglobin, N. Agmon and G.M. Sastry 212 (1996) 207
- Exploratory Pariser–Parr–Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357

- Experimental and theoretical study of the C_{1s} shakeup spectra from biphenyl and p-terphenyl, C. Enkvist, S. Lunell and S. Svensson 214 (1997) 123
- Poly-amino-enolates: first examples of odd alternant conducting polymers, A.J.W. Tol 215 (1997) 319
- Phenomenological model for reaction kinetics coupled to a relaxing environment, Y.A. Berlin, A.L. Burin and S.F. Fischer 220 (1997) 25
- Spectroscopic properties of chlorophylls and their derivatives. Influence of molecular structure on the electronic state, Y. Nonomura, S. Igarashi, N. Yoshioka and H. Inoue 220 (1997) 155
- Molecular aggregates*
- The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria, V.I. Novoderezhkin and A.P. Razjivin 211 (1996) 203
- Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye, M.A. Drobizhev, M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky 211 (1996) 455
- The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines, J.M. Warman, P.G. Schouten, G.H. Gelinck and M.P. de Haas 212 (1996) 183
- Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium–water clusters, J.C. Contador, M.A. Aguilar and F.J.O. del Valle 214 (1997) 113
- Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I, J. Zhang and M. Baumgarten 214 (1997) 291
- Calculation of triplet–singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs, K.M. Salikhov, J. Schlüpmann, M. Plato and K. Möbius 215 (1997) 23
- A study of the hydration of aluminate minerals based on the measurements of the mean and the variance of the proton magnetic resonance relaxation rate, A.B. Kudryavtsev, T.V. Kouznetsova, W. Linert and G. Hunter 215 (1997) 419
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81
- Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of $He-Cl_2$ and $Ar-Cl_2$, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 219 (1997) 161
- Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
- Effects of CCl_4 on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions, M.F. Ferreira Marques, H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre 220 (1997) 233
- Nonradiative processes and infrared emission in matrix isolated ND, N. Caspary, B.E. Wurfel, A.M. Smith and V.E. Bondybey 220 (1997) 241
- Degree of aggregation of indocyanine green in aqueous solutions determined by Mie scattering, R. Weigand, F. Rotermund and A. Penzkofer 220 (1997) 373
- J-aggregation and disaggregation of indocyanine green in water, F. Rotermund, R. Weigand and A. Penzkofer 220 (1997) 385

-dimers

- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- Structures and potential energy surface of Faujasitic zeolite/water, J. Limtrakul, P. Treesukol, C. Ebner, R. Sansone and M. Probst 215 (1997) 77
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81
- Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221
- Quantum chemical exploration of the HCl dimer interaction, A.W. Meredith, L. Ming and S. Nordholm 220 (1997) 63
- Forward and reverse excitation energy transport in concentrated two-component systems, P. Bojarski and L. Kuřak 220 (1997) 323

-van der Waals molecules

- Ab initio calculation of three-body interaction in the $(\text{H}_2)_3$ trimer, P. Wind and I. Røeggen 211 (1996) 179
- Potential energy curve of the $\text{XO}^+(^1\Sigma^+)$ ground state of HgAr determined from $\text{AO}^+(^3\Pi) \rightarrow \text{XO}^+$ and $\text{B1}(^3\Sigma^+) \rightarrow \text{XO}^+$ fluorescence spectra, J. Koperski 211 (1996) 191
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone–carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- Interaction forces and energy transfer dynamics of $\text{LiH}(^1\Sigma^+)$ and helium atoms. I. The ab initio evaluation of the lowest potential energy surface, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper 215 (1997) 227
- Interaction forces and energy transfer dynamics of $\text{LiH}(^1\Sigma^+)$ and helium atoms. II. Rotationally inelastic collisions and excitation efficiency, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi and M. Sironi 215 (1997) 239
- The van der Waals vibrational frequencies of the aniline–carbon monoxide complex in its S_1 state, J.-G. Jäckel, R. Schmid, H. Jones, T. Nakanaga and H. Takeo 215 (1997) 291
- Spin–orbit interaction in heavy group 13 atoms and TlAr , T. Leininger, A. Berning, A. Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad 217 (1997) 19
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Infrared spectroscopy of aniline–X ($\text{X} = \text{N}_2, \text{CH}_4, \text{CHF}_3, \text{CO}$) clusters and their corresponding cluster cations in the NH_2 -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Intermolecular vibrations of the van der Waals complex $\text{p-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$, Y. Hu, W. Lu and S. Yang 218 (1997) 325

- Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He-Cl₂ and Ar-Cl₂, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 219 (1997) 161
- Ab initio study of the structure, vibrational spectra and binding energy of HCl-CIO and Cl₂-CIO complexes, S. Aloisio and J.S. Francisco 219 (1997) 201
- clusters*
- Infrared spectroscopy of matrix-isolated carbon clusters, with emphasis on C₈ and C₉, J. Szczepanski, S. Ekern, C. Chapo and M. Vala 211 (1996) 359
- Photophysics and photochemistry of I₂ (D, D') in rare gas clusters, K.L. Randall and D.J. Donaldson 211 (1996) 377
- Solvent effects on sol-gel transition of alginate solutions by addition of cupric ions, H. Zheng, K. Jiang, Q. Zhang and J. Wang 211 (1996) 507
- Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence, V.F. Tarasov, H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob 212 (1996) 353
- Intracuster ion-molecule reactions induced by the synchrotron radiation in allyl bromide-ammonia clusters, C. Dedonder-Lardeux, C. Jouvet, S. Martrenchard-Barra, D. Solgadi, F. Talbot, M. Vervloet, I. Dimicoli and M. Richard-Viard 212 (1996) 371
- Spin-spin interactions in the reduced [Fe₆S₆]⁵⁺ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium-water clusters, J.C. Contador, M.A. Aguilar and F.J.O. del Valle 214 (1997) 113
- Electronic charge density transfer along a constrained reaction path from a hydronium ion configuration into a hydrogen chemisorption state on Cu(100), An.M. Kuznetsov and W. Lorenz 214 (1997) 243
- Double exchange in distorted trimeric mixed-valence clusters, M.I. Belinsky 215 (1997) 7
- Clusters containing BF₃, O(CH₃)₂ and aromatic compounds: An electron impact and photoionization study, C.G. Eisenhardt, S. Ring, H.-W. Jochims and H. Baumgärtel 216 (1997) 427
- Carbon-oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- A full quantum study of the vibrational predissociation mechanisms in Ar₃⁺ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Infrared spectroscopy of aniline-X (X = N₂, CH₄, CHF₃, CO) clusters and their corresponding cluster cations in the NH₂-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1
- C₉₀ temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
- Scattering of large argon clusters from a Pt(111) surface with low collision velocities, M. Svanberg, N. Marković and J.B.C. Pettersson 220 (1997) 137
- Nonradiative processes and infrared emission in matrix isolated ND, N. Caspary, B.E. Wurfel, A.M. Smith and V.E. Bondybey 220 (1997) 241

-complexes

- Irreversible random transition theory as applied to rate processes in condensed media: Transient effects of constrained configuration rearrangements in complex systems, Yu.A. Berlin 212 (1996) 29
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone–carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- A study of the 1B_2 excited state geometries of the metal–metal quadruply bonded compounds $Mo_2X_4(PMe_3)_4$ ($X = Cl, Br$ or I), C. Svendsen, M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark 215 (1997) 89
- Evaluation of luminescence decay measurements probed on pure and doped Pt(IV) hexahalogeno complexes I. Exponential rise time and decay curves applying various statistical tests, I. Biertümpel and H.-H. Schmidtke 215 (1997) 271
- Structure and selective visible photodissociation of the $O_3:Br_2$ and $O_3:BrCl$ complexes: an infrared matrix isolation and ab initio study, M. Bahou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 216 (1997) 105
- Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis–trans photoisomerization dynamics, G. Ponterini 216 (1997) 193
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O, N_2$ and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243
- Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
- Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H. Ågren 220 (1997) 79

Free radicals (including hydronium and muonium)

- Experimental and theoretical study of the recombination reaction of $FC(O)O$ radicals, A.E. Croce, C.J. Cobos and E. Castellano 211 (1996) 215
- Magnetic field dependent yield of geminate radical pair recombination in micelles. Effect of intraradical spin lattice relaxation, J.S. Jørgensen, J.B. Pedersen and A.I. Shushin 211 (1996) 235
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study, A. Richter, H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig 214 (1997) 321
- Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region, A. Fahr, P. Hassanzadeh, B. Laszlo and R.E. Huie 215 (1997) 59
- Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra, A.M. Mebel and S.-H. Lin 215 (1997) 329
- Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives, V.L. Vyazovkin and V.A. Tolkathev 216 (1997) 135
- Theoretical study of cyclic radicals NO_x ($x = 2–6$), Y. Li and S. Iwata 219 (1997) 209
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355

Quasiparticles (including excitons)

- Remote ionization and recombination through the multichannel electron transfer, A.I. Burshtein and P.A. Frantsuzov 212 (1996) 137
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Ultracold atoms in modulated standing light waves, K. Drese and M. Holthaus 217 (1997) 201

Defects and impurities

- Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er^{3+} in YVO_4 , J.A. Capobianco, P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli 214 (1997) 329
- Electron paramagnetic resonance of Ni(II) doped tris(ethylenediamine)zinc(II) dinitrate, C.R. Wilson, M.J. Riley, D. Wang and G.R. Hanson 217 (1997) 63
- Dynamical simulation of the driven spin-boson system: The influence of interblip correlations, M. Winterstetter and U. Weiss 217 (1997) 155
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

Ions and charge carriers

- A Kramers reaction rate theory for electrochemical ion transfer reactions, M.T.M. Koper and W. Schmickler 211 (1996) 123
- Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique, F.F. Brazgun, V.A. Nadochenko, I.V. Rubtsov and L.V. Lukin 211 (1996) 469
- Remote ionization and recombination through the multichannel electron transfer, A.I. Burshtein and P.A. Frantsuzov 212 (1996) 137
- Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na_2O , V.M. Syutkin and V.A. Tolkatchev 212 (1996) 149
- The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines, J.M. Warman, P.G. Schouten, G.H. Gelinck and M.P. de Haas 212 (1996) 183
- Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state, P. Karafiloglou 214 (1997) 171
- Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study, A. Richter, H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig 214 (1997) 321
- Drift velocity of ions in lighter gases in electric and magnetic fields, L. Ferrari and A. Carbognani 215 (1997) 37
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation, W. Lorenz, M. Handschuh and F. Bergmann 215 (1997) 139
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions, F. Bergmann, M. Handschuh and W. Lorenz 215 (1997) 157
- The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory, A. Beghin and T. Stoecklin 215 (1997) 261

- Inelastic neutron scattering studies of polyanilines and partially deuterated analogues, F. Fillaux, N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colomban, A. Gruger, A. Régis and L.T. Yu 216 (1997) 281
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Diatomics-in-molecules study of the ground and excited states of H_3^- , A.K. Belyaev and A.S. Tiukanov 220 (1997) 43

Phenomena

Molecular structure

- Spin-orbit effects in fullerenes, F.J. Adrian 211 (1996) 73
- Ab initio calculations of the rovibrational states of He_2N^{2+} , J.M. Hughes and E.I. von Nagy-Felsobuki 211 (1996) 135
- Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives, A. Broo and A. Holmén 211 (1996) 147
- The dissociation energies of FeF, FeCl, and FeBr and their positive ions, C.W. Bauschlicher Jr. 211 (1996) 163
- Potential energy curve of the $X0^+(^1\Sigma^+)$ ground state of HgAr determined from $A0^+(^3\Pi) \rightarrow X0^+$ and $B1(^3\Sigma^+) \rightarrow X0^+$ fluorescence spectra, J. Koperski 211 (1996) 191
- Interstellar silicon–nitrogen chemistry. I. The microwave and the infrared signatures of the HSiN, HNSi, HSiNH₂, HNSiH₂ and HSiNH⁺ species, O. Parisel, M. Hanus and Y. Ellinger 212 (1996) 331
- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC₄H₂, HC₃NH, and HC₃O, H. Wang and A.L. Cooksy 213 (1996) 139
- Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state, P. Karafiloglou 214 (1997) 171
- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the FCO + H₂ → HFCO + H abstraction reaction, J.S. Francisco 214 (1997) 213
- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the FCO + H₂ → HFCO + H abstraction reaction, J.S. Francisco 214 (1997) 213
- Ab initio calculations of S₁ excited state vibrational spectra of benzene, naphthalene and anthracene, G.S. Jas and K. Kuczera 214 (1997) 229
- A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices, J. Kölm, A. Engdahl, O. Schrems and B. Nelander 214 (1997) 313
- Hybridizations of fullerenes: their relations with properties and applications in computation, X.P. Yu, Z.L. Cao and R.S. Han 215 (1997) 1
- Poly-amino-enolates: first examples of odd alternant conducting polymers, A.J.W. Tol 215 (1997) 319
- Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra, A.M. Mebel and S.-H. Lin 215 (1997) 329
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81

- Spin-orbit interaction in heavy group 13 atoms and TlAr, T. Leininger, A. Berning, A. Nicklass, H. Stoll, H.-J. Werner and H.-J. Flad 217 (1997) 19
- Carbon-oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran-argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
- C₉₀ temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
- Ab initio study of the structure, vibrational spectra and binding energy of HCl-ClO and Cl₂-ClO complexes, S. Aloisio and J.S. Francisco 219 (1997) 201
- Theoretical study of cyclic radicals NO_x (x = 2–6), Y. Li and S. Iwata 219 (1997) 209
- The relationship between the molecular structure of semiquinone radicals and their g-values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291
- Diatomics-in-molecules study of the ground and excited states of H₃⁺, A.K. Belyaev and A.S. Tiukanov 220 (1997) 43
- Spectroscopic properties of chlorophylls and their derivatives. Influence of molecular structure on the electronic state, Y. Nonomura, S. Igarashi, N. Yoshioka and H. Inoue 220 (1997) 155
- Degree of aggregation of indocyanine green in aqueous solutions determined by Mie scattering, R. Weigand, F. Rotermund and A. Penzkofer 220 (1997) 373
- Vibrations and rotations of molecules*
- Selective rovibrational energy transfer: A classical trajectory study of collisional energy redistribution in methyl radical, G.S. Peng and R.P. Parson 211 (1996) 17
- Ab initio calculations of the rovibrational states of He₂N²⁺, J.M. Hughes and E.I. von Nagy-Felsobuki 211 (1996) 135
- An improved classical approach quantum encounter treatment of collision-induced vibrational energy transfer. Application to He + CO (n_i = 1, 2), N. Marković, T.D. Sewell, S. Nordholm and A. Miklavc 211 (1996) 277
- Infrared spectroscopy of matrix-isolated carbon clusters, with emphasis on C₈ and C₉, J. Szczepanski, S. Ekern, C. Chappo and M. Vala 211 (1996) 359
- Fast-ion beam laser spectroscopy of ¹⁴N₂⁺ and ¹⁵N₂⁺: high-resolution study of the (1, 2) band of the B ²Σ_u⁺–X ²Σ_g⁺ system, K. Boudjarane, A. Alikacem and M. Larzillière 211 (1996) 393
- Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam, A. Obrebski, T. Kaps and U. Cerny 212 (1996) 311
- Interstellar silicon-nitrogen chemistry. I. The microwave and the infrared signatures of the HSiN, HNSi, HSiNH₂, HNSiH₂ and HSiNH⁺ species, O. Parisel, M. Hanus and Y. Ellinger 212 (1996) 331
- Vibrational spectrum of the K-590 intermediate in the bacteriorhodopsin photocycle at room temperature: picosecond time-resolved resonance coherent anti-Raman spectroscopy, L. Ujj, F. Jäger, A. Popp and G.H. Atkinson 212 (1996) 421
- Vibrational structure of the BrCN⁺ ion from high resolution photoelectron spectroscopy, J.H.D. Eland, P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson 212 (1996) 457
- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17

- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejski, G. Waliszewska and H. Abramczyk 213 (1996) 341
- The anharmonic effect as originated from the asymmetry of a rotor. The case study of an asymmetric rotor coupled with a simple harmonic oscillator, G. Wu 214 (1997) 15
- An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen, V. Sreedhara Rao and A.K. Chandra 214 (1997) 103
- Ab initio calculations of S_1 excited state vibrational spectra of benzene, naphthalene and anthracene, G.S. Jas and K. Kuczera 214 (1997) 229
- Tunnelling of the one-dimensional rotor NH_3D^+ in the NH_4ClO_4 and NH_4PF_6 lattices, H.G. Büttner, G.J. Kearley and B. Frick 214 (1997) 425
- Rotational and vibrational excitation of the N_2^+ (B) state in a He + N_2 electron-beam plasma, A.E. Belikov 215 (1997) 97
- Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters, R.G. Schmidt, M.C. Böhm and J. Brickmann 215 (1997) 207
- Rotation/precession of NH_3 groups in Hofmann clathrates, M. Neumann and G.J. Kearley 215 (1997) 253
- Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra, A.M. Mebel and S.-H. Lin 215 (1997) 329
- The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid, M.R. Johnson, M. Neumann, B. Nicolai, P. Smith and G.J. Kearley 215 (1997) 343
- Matrix isolation and theoretical studies of ONNO: Assignment of a new combination band and density functional calculations, J.F. Canty, E.G. Stone, S.B.H. Bach and D.W. Ball 216 (1997) 81
- Sol-gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis, S.M. Arabei, S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup 216 (1997) 163
- Fine-structure dependence of the $Ar^*(^3P_{0,2}) + N_2(X)$ excitation transfer process, E.J.D. Vredenburg, W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 259
- $Ar^*(^3P_2)/Kr^*(^3P_{0,2}) + N_2(X)$ excitation transfer collisions: final state rotational alignment, E.J.D. Vredenburg, W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 273
- Effect of strong excitation of the CO_2 asymmetric mode on transport properties, A. Chikhaoui and E.V. Kustova 216 (1997) 297
- Vibronic theory of electric hysteresis in "bistable" mixed-valence molecular salts, K. Boukheddaden and F. Varret 216 (1997) 373
- A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH, X. Chapuisat, C. Saint-Espès, C. Zuhrt and L. Zülicke 217 (1997) 43
- The phosphorescence excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione, A.A. Ruth, F.J. O'Keeffe, R.P. Brint and M.W.D. Mansfield 217 (1997) 83

- Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury, P. Backhaus and B. Schmidt 217 (1997) 131
- Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule, H. Dietz, A. Materny and V. Engel 217 (1997) 249
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Intermolecular vibrations of the van der Waals complex $p\text{-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$, Y. Hu, W. Lu and S. Yang 218 (1997) 325
- Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
- Ab initio study of the structure, vibrational spectra and binding energy of $\text{HCl}\text{--}\text{ClO}$ and $\text{Cl}_2\text{--}\text{ClO}$ complexes, S. Aloisio and J.S. Francisco 219 (1997) 201
- Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221
- Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
- Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305
- Strong-field approach to ultrafast pump–probe spectra: dye molecules in solution, D.H. Schirrmeister and V. May 220 (1997) 1
- Spectroscopic investigation of ground state pyrrole ($^{12}\text{C}_4\text{H}_5\text{N}$): the N–H stretch, A. Mellouki, R. Georges, M. Herman, D.L. Snavely and S. Leytner 220 (1997) 311

Electronic structure and states

- Correlated electronic potential-energy surfaces for proton interactions with N_2 , F.A. Gianturco, S. Kumar and F. Schneider 211 (1996) 33
- Pressure effects on the $\text{Cl}_2(\text{D}'\text{--}\text{A}')$ transition at 258 nm, J.B. Nee and S. Hubinger 211 (1996) 403
- Single molecule polarization spectroscopy: pentacene in p-terphenyl, F. Güttler, M. Croci, A. Renn and U.P. Wild 211 (1996) 421
- Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine, Y. Zheng, C.E. Brion, M.J. Brunger, K. Zhao, A.M. Grisogono, S. Braidwood, E. Weigold, S.J. Chakravorty, E.R. Davidson, A. Sgamellotti and W. von Niessen 212 (1996) 269
- Interstellar silicon–nitrogen chemistry. I. The microwave and the infrared signatures of the HSiN , HNSi , HSiNH_2 , HNSiH_2 and HSiNH^+ species, O. Parisel, M. Hanus and Y. Ellinger 212 (1996) 331
- Ab initio study on the electronic structure of the $4^2\Sigma^+$ and $5^2\Sigma^+$ excited states of CO^+ , N. Honjou and E. Miyoshi 212 (1996) 363
- An ab initio perturbed ion study of structural properties of TiO_2 , SnO_2 and GeO_2 rutile lattices, A.C. Camargo, J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés 212 (1996) 381
- Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR, N.A. Salih, O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen 212 (1996) 409

- Vibrational structure of the BrCN^+ ion from high resolution photoelectron spectroscopy, J.H.D. Eland, P. Baltzer, M. Lundqvist, B. Wannberg and L. Karlsson 212 (1996) 457
- A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability, F. Varret, J. Linares and K. Boukheddaden 212 (1996) 487
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- The formalism and matrix elements of a complete potential-harmonic scheme for directly solving the Schrödinger equation of the helium atom, Y.-X. Wang and C.-H. Deng 214 (1997) 33
- Experimental and theoretical study of the C_{18} shakeup spectra from biphenyl and p-terphenyl, C. Enkvist, S. Lunell and S. Svensson 214 (1997) 123
- The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel 214 (1997) 191
- Calculation of ground- and excited-state potential energy curves for the Hg_2 molecule in a pseudopotential approach, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss 214 (1997) 277
- Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I, J. Zhang and M. Baumgarten 214 (1997) 291
- Charge-transfer states and the band gap in crystalline fullerene, A. Eilmes, R.W. Munn, B. Pac and P. Petelenz 214 (1997) 341
- Ultraviolet absorption and cross sections of propargyl (C_3H_3) radicals in the 230–300 nm region, A. Fahr, P. Hassanzadeh, B. Laszlo and R.E. Huie 215 (1997) 59
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation, W. Lorenz, M. Handschuh and F. Bergmann 215 (1997) 139
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions, F. Bergmann, M. Handschuh and W. Lorenz 215 (1997) 157
- Theoretical study of the low-lying excited states of ABCO, DABCO and homologous cage amines, V. Galasso 215 (1997) 183
- Imaging of the HOMO electron density in $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ by electron momentum spectroscopy: a comparison with Hartree–Fock and DFT calculations, J. Rolke, Y. Zheng, C.E. Brion, S.J. Chakravorty, E.R. Davidson and I.E. McCarthy 215 (1997) 191
- Interaction forces and energy transfer dynamics of LiH ($^1\Sigma^+$) and helium atoms. I. The ab initio evaluation of the lowest potential energy surface, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper 215 (1997) 227
- Charge-transfer excitons in the dielectric theory of molecular crystals, R.W. Munn 215 (1997) 301
- Poly-amino-enolates: first examples of odd alternant conducting polymers, A.J.W. Tol 215 (1997) 319
- Matrix-isolated oxygen: line-shapes and transition probabilities of the $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$, $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ and $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transitions, G. Tyczkowski, U. Schurath, M. Bodenbinder and H. Willner 215 (1997) 379
- Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3 : absolute oscillator strengths and dipole-induced breakdown pathways, J.W. Au, G. Cooper and C.E. Brion 215 (1997) 397

- Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn–Teller distortion in the excited electronic state on Raman intensities, H. Torii, M. Tasumi, I.M. Bell and R.J.H. Clark 216 (1997) 67
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases, M. Pulfer, C.-H. Hu and D.P. Chong 216 (1997) 91
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules, C.-H. Hu and D.P. Chong 216 (1997) 99
- Analysis of the $D'2_g - A'2_u$ transition in the molecular iodine by laser-induced-fluorescence Fourier-transform spectrometry, D. Cerny, R. Bacis, S. Churassy, D. Inard, M. Lamrini and M. Nota 216 (1997) 207
- A quasi-atomic treatment of chemical and structural effects on K-shell excitations in hexagonal and cubic BN crystals, R. Franke, S. Bender, J. Hormes, A.A. Pavlychev and N.G. Fominych 216 (1997) 243
- Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree–Fock method, F.E. Jorge, E.V.R. de Castro and A.B.F. da Silva 216 (1997) 317
- Crystal structure and photoluminescence of single crystals of fullerene–9,9'-*trans*-bis(teluraxanthenyl) molecular complex: $C_{26}H_{18}Te_2 \cdot C_{60} \cdot CS_2$, V.V. Kveder, E.A. Steinman, B.Zh. Narymbetov, S.S. Khasanov, L.P. Rozenberg, R.P. Shibaeva, A.V. Bazhenov, A.V. Gorbunov, M.Yu. Maksimuk, D.V. Konarev, R.N. Lyubovskaya and Yu.A. Ossipyan 216 (1997) 407
- Electron paramagnetic resonance of Ni(II) doped tris(ethylenediamine)zinc(II) dinitrate, C.R. Wilson, M.J. Riley, D. Wang and G.R. Hanson 217 (1997) 63
- Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
- Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G. Granucci and M. Persico 219 (1997) 21
- Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
- A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 , D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
- Theoretical study of cyclic radicals NO_x ($x = 2-6$), Y. Li and S. Iwata 219 (1997) 209
- Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
- Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ ($XY \equiv FCl, Cl_2, FH$), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J.

- Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
- Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341
- Photoacoustic spectra of BaFBr:Eu²⁺ phosphors, Y. Zhang 219 (1997) 353
- VUV optical-absorption and electron-energy-loss spectroscopy of formamide, J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker and M.R.F. Siggel 220 (1997) 191
- Classification of Cm I energy levels using PCA-BPN and PCA-NLM, X. Cao, H. Liu and N. Chen 220 (1997) 289
- Extended Fenske–Hall LCAO MO calculations of core-level shifts in solid P compounds, R. Franke, T. Chassé, J. Reinhold, P. Streubel and R. Szargan 220 (1997) 299
- Electric and magnetic properties*
- Spin–orbit effects in fullerenes, F.J. Adrian 211 (1996) 73
- Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na₂O, V.M. Syutkin and V.A. Tolkatchev 212 (1996) 149
- Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR, N.A. Salih, O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen 212 (1996) 409
- Spin–spin interactions in the reduced [Fe₆S₆]⁵⁺ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- On the calculation of hydrogen NMR chemical shielding, D.B. Chesnut 214 (1997) 73
- The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH[−] and OH[−]·H₂O, S.P.A. Sauer, V. Špirko, I. Paidarová and W.P. Kraemer 214 (1997) 91
- Electronic charge density transfer along a constrained reaction path from a hydronium ion configuration into a hydrogen chemisorption state on Cu(100), An.M. Kuznetsov and W. Lorenz 214 (1997) 243
- Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I, J. Zhang and M. Baumgarten 214 (1997) 291
- Charge-transfer states and the band gap in crystalline fullerene, A. Eilmès, R.W. Munn, B. Pac and P. Petelenz 214 (1997) 341
- Influence of rotational diffusion on the electric field induced effect on the fluorescence spectrum of diluted solutions. I. Theory and numerical simulations, H. Reis and W. Baumann 214 (1997) 383
- Hybridizations of fullerenes: their relations with properties and applications in computation, X.P. Yu, Z.L. Cao and R.S. Han 215 (1997) 1
- Double exchange in distorted trimeric mixed-valence clusters, M.I. Belinsky 215 (1997) 7
- Drift velocity of ions in lighter gases in electric and magnetic fields, L. Ferrari and A. Carbognani 215 (1997) 37
- Dipole polarizability and hyperpolarizability of FCN, ClCN, BrCN and ICN, G. Maroulis and C. Pouchan 215 (1997) 67
- Cotton–Mouton effect and shielding polarizabilities of ethylene: an MCSCF study, S. Coriani, A. Rizzo, K. Ruud and T. Helgaker 216 (1997) 53

- Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation, J.M. Luis, J. Martí, M. Duran and J.L. Andrés 217 (1997) 29
- Electron paramagnetic resonance of Ni(II) doped tris(ethylenediamine)zinc(II) dinitrate, C.R. Wilson, M.J. Riley, D. Wang and G.R. Hanson 217 (1997) 63
- Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH⁻ and NeH⁺, J. Vojtík and J. Fišer 218 (1997) 13
- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43
- The magnetic field influence on bridge-assisted electron transfer, E.G. Petrov, I.S. Tolokh, V.V. Gorbach and V. May 220 (1997) 249
- Spin splittings*
- Spin-correlated radical pairs in micellar systems: mechanism of CIDEP and the micelle size dependence, V.F. Tarasov, H. Yashiro, K. Maeda, T. Azumi and I.A. Shkrob 212 (1996) 353
- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H₂, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309
- Optical activity*
- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465
- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- Molecular interactions*
- Ab initio calculation of three-body interaction in the (H₂)₃ trimer, P. Wind and I. Røeggen 211 (1996) 179
- Generalized oscillator strengths for SF₆ in the S 2p inner-shell region, Z. Felfli, I. Fomunung, D. Bessis and A.Z. Msezane 211 (1996) 325
- Order parameters and carbon shielding tensors of bis-MSB from ¹³C NMR measurements in a nematic liquid crystal, R. Tarroni and C. Zannoni 211 (1996) 337
- Photophysics and photochemistry of I₂ (D, D') in rare gas clusters, K.L. Randall and D.J. Donaldson 211 (1996) 377
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejki, G. Waliszewska and H. Abramczyk 213 (1996) 341
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413

- Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium–water clusters, J.C. Contador, M.A. Aguilar and F.J.O. del Valle 214 (1997) 113
- Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures, A. Baranowski, K. Jerie and J. Gliński 214 (1997) 143
- A new potential for the description of intermolecular interactions for rigid biaxial molecules, V.V. Ginzburg, M.A. Glaser and N.A. Clark 214 (1997) 253
- Structures and potential energy surface of Faujasitic zeolite/water, J. Limtrakul, P. Treesukol, C. Ebner, R. Sansone and M. Probst 215 (1997) 77
- On the $O_2(v') + O_2(v'')$ atmospheric reaction: a quasiclassical trajectory study, A.J.C. Varandas and W. Wang 215 (1997) 167
- Interaction forces and energy transfer dynamics of $LiH(^1\Sigma^+)$ and helium atoms. I. The ab initio evaluation of the lowest potential energy surface, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi, M. Sironi, J. Gerratt and D.L. Cooper 215 (1997) 227
- Sol–gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion, S.G. Kulikov, A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot 216 (1997) 147
- Ion pairing of bisdimethylamino pentamethinecyanine perchlorate and its consequences on the cis–trans photoisomerization dynamics, G. Ponterini 216 (1997) 193
- Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose, B. Leroux, H. Bizot, J.W. Brady and V. Tran 216 (1997) 349
- Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion, H. Hulsman 217 (1997) 107
- Infrared spectroscopy of aniline–X ($X = N_2, CH_4, CHF_3, CO$) clusters and their corresponding cluster cations in the NH_2 -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
- Statistical mechanical treatment of reactive solvent extraction, M. Lukhezo, L.J. Dunne, B.G. Reuben and M.S. Verrall 220 (1997) 53
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H. Ågren 220 (1997) 79
- J-aggregation and disaggregation of indocyanine green in water, F. Rotermund, R. Weigand and A. Penzkofer 220 (1997) 385

Spectral bandshapes and intensities

- Maximum entropy imaging and quantum molecular timescale generalized Langevin equation theory, H.K. McDowell and A.M. Clogston 211 (1996) 91
- Absorption cross section measurements of water vapor in the wavelength region 120 to 188 nm, K. Yoshino, J.R. Esmond, W.H. Parkinson, K. Ito and T. Matsui 211 (1996) 387
- Comments on the mode coupling theory for structural relaxation, W. Götze and L. Sjögren 212 (1996) 47
- The charge transfer state of excited bianthryl and a derivative: solvatochromism, emission CT spectra broadening in homogeneous solvents, H. Laguitton-Pasquier, R. Pansu, J.-P. Chauvet, A. Collet, J. Faure and R. Lapouyade 212 (1996) 437
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181

- Interatomic potentials for XO^+ and B^31 states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- A study of the 1B_2 excited state geometries of the metal–metal quadruply bonded compounds $Mo_2X_4(PMe_3)_4$ ($X = Cl, Br$ or I), C. Svendsen, M.J. Nielsen, O.S. Mortensen, S.J.R. Allers and R.J.H. Clark 215 (1997) 89
- Matrix-isolated oxygen: line-shapes and transition probabilities of the $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$, $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ and $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transitions, G. Tyczkowski, U. Schurath, M. Bodenbinder and H. Willner 215 (1997) 379
- Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3 : absolute oscillator strengths and dipole-induced breakdown pathways, J.W. Au, G. Cooper and C.E. Brion 215 (1997) 397
- A quasi-atomic treatment of chemical and structural effects on K-shell excitations in hexagonal and cubic BN crystals, R. Franke, S. Bender, J. Hormes, A.A. Pavlychev and N.G. Fominykh 216 (1997) 243
- Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p, 2s; Cl 2p, 2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
- Collision-induced electronic transitions in complexes between benzene and molecular oxygen, B.F. Minaev, K.V. Mikkelsen and H. Ågren 220 (1997) 79
- Coupling of electronic and nuclear motion*
- Stochastic wave packet vs. direct density matrix solution of Liouville–von Neumann equations for photodesorption problems, P. Saalfrank 211 (1996) 265
- An investigation of the photodissociation of molecular oxygen in the 75 to 85 nm region, A.L. Jones, A.J. Blake, L. Torop and D.G. McCoy 211 (1996) 291
- Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye, M.A. Drobizhev, M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky 211 (1996) 455
- A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability, F. Varret, J. Linares and K. Boukheddaden 212 (1996) 487
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- Ab initio determination of quasi-diabatic states for multiple reaction pathways, P. Cattaneo and M. Persico 214 (1997) 49
- The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH^- and $OH^- \cdot H_2O$, S.P.A. Sauer, V. Špirko, I. Paidarová and W.P. Kraemer 214 (1997) 91

- Sol-gel hosts doped with porphyrin derivatives. Part I. Spectroscopy, hole-burning and spectral diffusion, S.G. Kulikov, A.V. Veret-Lemarinier, J.P. Galaup, F. Chaput and J.P. Boilot 216 (1997) 147
- Inelastic neutron scattering studies of polyanilines and partially deuterated analogues, F. Fillaux, N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colombar, A. Gruger, A. Régis and L.T. Yu 216 (1997) 281
- Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule, H. Dietz, A. Materny and V. Engel 217 (1997) 249
- Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach, B. Wolfseder, L. Seidner, G. Stock and W. Domcke 217 (1997) 275
- Energy transfer processes*
- Selective rovibrational energy transfer: A classical trajectory study of collisional energy redistribution in methyl radical, G.S. Peng and R.P. Parson 211 (1996) 17
- Correlated electronic potential-energy surfaces for proton interactions with N₂, F.A. Gianturco, S. Kumar and F. Schneider 211 (1996) 33
- The theory of Forster-type migration between clusters of strongly interacting molecules: application to light-harvesting complexes of purple bacteria, V.I. Novoderezhkin and A.P. Razjivin 211 (1996) 203
- An improved classical approach quantum encounter treatment of collision-induced vibrational energy transfer. Application to He + CO ($n_i = 1, 2$), N. Marković, T.D. Sewell, S. Nordholm and A. Miklavc 211 (1996) 277
- Translational spectroscopy of H⁻ produced by collision induced dissociation of H₃⁺ on He, H. Martinez and A. Amaya-Tapia 211 (1996) 299
- Reaction path Hamiltonian analysis of the dynamics for Cl⁻ + CH₃Br → ClCH₃ + Br⁻ S_N2 nucleophilic substitution, H. Wang and W.L. Hase 212 (1996) 247
- Development and interconnections of the temperatures in the translational, rotational and vibrational degrees of freedom in a potassium monomer/dimer beam, A. Obrebski, T. Kaps and U. Cerny 212 (1996) 311
- A partially ergodic multiple encounter theory of collisional energy transfer, L.E.B. Börjesson and S. Nordholm 212 (1996) 393
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- The anharmonic effect as originated from the asymmetry of a rotor. The case study of an asymmetric rotor coupled with a simple harmonic oscillator, G. Wu 214 (1997) 15
- Dispersive transport of triplet excitation of benzaldehyde in solid ethanol solution, S.A. Bagnich 214 (1997) 351
- Reported blue upconversion from U⁴⁺ doped into Cs₂ZrCl₆ single crystals under green laser excitation, P.A. Tanner, J. Dexpert-Ghys, Z.W. Pei and J. Lin 215 (1997) 125
- Femtosecond dynamics of excited states in sexithiophene thin films, G. Klein, C. Jundt, B. Sipp, A.A. Villaeys, A. Boeglin, A. Yassar, G. Horowitz and F. Garnier 215 (1997) 131

- Interaction forces and energy transfer dynamics of $\text{LiH}(^1\Sigma^+)$ and helium atoms. II. Rotationally inelastic collisions and excitation efficiency, F.A. Gianturco, S. Kumar, S.K. Pathak, M. Raimondi and M. Sironi 215 (1997) 239
- Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA, V.V. Eremenko, V.A. Karachevtsev and V.V. Slavin 216 (1997) 1
- Nonequilibrium distributions of rotational and vibrational energies in a free-jet expansion, H. Hulsman 217 (1997) 107
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
- Strong-field approach to ultrafast pump–probe spectra: dye molecules in solution, D.H. Schirmer and V. May 220 (1997) 1
- Scattering of large argon clusters from a Pt(111) surface with low collision velocities, M. Svanberg, N. Marković and J.B.C. Pettersson 220 (1997) 137
- Forward and reverse excitation energy transport in concentrated two-component systems, P. Bojarski and L. Kuřak 220 (1997) 323

Molecular photophysical processes

- Higher excited-state triplet–singlet intersystem crossing of some organic dyes, S. Reindl and A. Penzkofer 211 (1996) 431
- Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model, C. Scharnagl and S.F. Fischer 212 (1996) 231
- The charge transfer state of excited bianthryl and a derivative: solvatochromism, emission CT spectra broadening in homogeneous solvents, H. Laguiton-Pasquier, R. Pansu, J.-P. Chauvet, A. Collet, J. Faure and R. Lapouyade 212 (1996) 437
- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore–protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Ab initio determination of quasi-diabatic states for multiple reaction pathways, P. Cattaneo and M. Persico 214 (1997) 49
- Ab initio calculations of electronic spectra of H_2S and H_2S_2 , M. Pericou-Cayere, M. Gelize and A. Dargelos 214 (1997) 81
- Photophysics of 4-dimethylamino 4'-cyanostilbene and model compounds: dual excited states revealed by sub-picosecond transient absorption and Kerr ellipsometry, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade and C. Rullière 214 (1997) 409
- Spectroscopy and photophysics of $\text{C}_{60}\text{H}_{18}$ and $\text{C}_{60}\text{H}_{36}$, R.V. Bensasson, T.J. Hill, E.J. Land, S. Leach, D.J. McGarvey, T.G. Truscott, J. Ebenhoch, M. Gerst and C. Rüchardt 215 (1997) 111
- Charge-transfer excitons in the dielectric theory of molecular crystals, R.W. Munn 215 (1997) 301
- Simultaneous control of selectivity and yield of molecular dissociation. Pulsed incoherent interference control, M. Shapiro, Z. Chen and P. Brumer 217 (1997) 325
- Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87

- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- Intramolecular dynamics*
- Molecular dynamics simulations of cis–trans isomerization for a proline-containing tripeptide in solution, S.Z. Wan, C.X. Wang, Y.W. Xu and Y.Y. Shi 211 (1996) 227
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- Dynamic effects in non-adiabatic charge transfer, E. Gudowska-Nowak 212 (1996) 115
- Dielectric relaxation models applied to the dynamics of myoglobin as determined by Mössbauer spectroscopy, I. Chang, H. Hartmann, Yu. Krupyanskii, A. Zharikov and F. Parak 212 (1996) 221
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- A weak-mode representation of floppy molecules. Part IV. Spectroscopic states of model HCN and CNH, X. Chapuisat, C. Saint-Espès, C. Zuhrt and L. Zülicke 217 (1997) 43
- A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables, Y. Watanabe, H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura 217 (1997) 317
- A simulation of ultrafast state-selective IR-laser-controlled isomerization of hydrogen cyanide based on global 3D ab initio potential and dipole surfaces, W. Jakubetz and B.L. Lan 217 (1997) 375
- Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279
- Ionization and fragmentation of OCS and CS_2 after photoexcitation around the sulfur 2p edge, U. Ankerhold, B. Esser and F. von Busch 220 (1997) 393
- radiationless transitions*
- Optical potential discrete variable representation method applied to the three-dimensional calculations of NeICl predissociation resonances, M. Monnerville and J.-M. Robbe 211 (1996) 249
- Vibron-mediated electronic relaxation in crystalline chlorine, D. Logan, C.A. Wight and V.A. Apkarian 217 (1997) 99
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355
- Ionization and fragmentation of OCS and CS_2 after photoexcitation around the sulfur 2p edge, U. Ankerhold, B. Esser and F. von Busch 220 (1997) 393
- vibrational energy redistribution (including vibrational dissociation)*
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111

- On the $O_2(v') + O_2(v'')$ atmospheric reaction: a quasiclassical trajectory study, A.J.C. Varandas and W. Wang 215 (1997) 167
- Control of tunneling processes with an external field in a four-level system: an analytic approach, R.I. Cukier, C. Denk and M. Morillo 217 (1997) 179
- A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Strong-field approach to ultrafast pump–probe spectra: dye molecules in solution, D.H. Schirrneister and V. May 220 (1997) 1
- Luminescence spectra, yields and lifetimes*
- The orientation of the transition dipole moments of TMA-DPH embedded in a poly(vinylalcohol) film, J.M. Muller, D.H. Harryvan, J.C.D. Verhagen, G. van Ginkel and E.E. van Faassen 211 (1996) 413
- Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans–cis photoisomerisation, Yu.V. Il'ichev, W. Kühnle and K.A. Zachariasse 211 (1996) 441
- Time-resolved electroluminescence from single and bilayer LEDs based upon substituted poly-arylenevinyls, Y.-H. Tak, H. Vestweber, H. Bässler, A. Bleyer, R. Stockmann and H.-H. Hörhold 212 (1996) 471
- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore–protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
- Optical spectroscopy, fluorescence dynamics and crystal-field analysis of Er^{3+} in YVO_4 , J.A. Capobianco, P. Kabro, F.S. Ermeneux, R. Moncorgé, M. Bettinelli and E. Cavalli 214 (1997) 329
- Reported blue upconversion from U^{4+} doped into Cs_2ZrCl_6 single crystals under green laser excitation, P.A. Tanner, J. Dexpert-Ghys, Z.W. Pei and J. Lin 215 (1997) 125
- Evaluation of luminescence decay measurements probed on pure and doped Pt(IV) hexahalogeno complexes I. Exponential rise time and decay curves applying various statistical tests, I. Biertümpel and H.-H. Schmidtke 215 (1997) 271
- Phonon thermoactivated exciton tunneling in crystals of weak charge transfer complexes N-TCPA doped with Nd8-TCPA, V.V. Eremenko, V.A. Karachevtsev and V.V. Slavin 216 (1997) 1
- Sol–gel hosts doped with porphyrin derivatives. Part II. Site selection spectra and vibronic analysis, S.M. Arabei, S.G. Kulikov, A.V. Veret-Lemarinier and J.P. Galaup 216 (1997) 163
- Vibron-mediated electronic relaxation in crystalline chlorine, D. Logan, C.A. Wight and V.A. Apkarian 217 (1997) 99
- Non-exponential decays of the S_1 vibronic levels of acetaldehyde, S.-H. Lee and I.-C. Chen 220 (1997) 175
- Coherence loss processes*
- Kohlrausch relaxation in electronic and molecular glasses, J.C. Phillips 212 (1996) 41
- Control of tunneling processes with an external field in a four-level system: an analytic approach, R.I. Cukier, C. Denk and M. Morillo 217 (1997) 179
- Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases, M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin and N.F. Scherer 217 (1997) 259
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355

Non-linear responses (including optical)

- Rydberg basis set effects on ab initio second hyperpolarizabilities of H_2 , C_6H_6 and CS_2 molecules, T. Hamada 211 (1996) 171
- Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques, P.C. Ray, N. Munichandrahiah and P.K. Das 211 (1996) 499
- Exploratory Pariser–Parr–Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- Time resolved spectroscopy of nonlinear solvation with pulses longer than electronic dephasing, B.D. Fainberg and B. Zolotov 216 (1997) 7
- Increase and saturation of the third order hyperpolarizabilities in homologous series of symmetric cyanines, W. Werncke, M. Pfeiffer, T. Johr, A. Lau, W. Grahn, H.-H. Johannes and L. Dähne 216 (1997) 337
- Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation, J.M. Luis, J. Martí, M. Duran and J.L. Andrés 217 (1997) 29
- Theoretical study of multiple high-order harmonic generation by intense ultrashort pulsed laser fields: A new generalized pseudospectral time-dependent method, X.-M. Tong and S.-I. Chu 217 (1997) 119
- Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations, M. Grifoni, L. Hartmann and P. Hänggi 217 (1997) 167
- Photodissociation of Ar_2^+ in strong laser fields, P. Schwendner, F. Seyl and R. Schinke 217 (1997) 233
- Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
- Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341
- Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects, S.J. Zilker and D. Haarer 220 (1997) 167

Multiphoton phenomena

- The van der Waals vibrational frequencies of the aniline–carbon monoxide complex in its S_1 state, J.-G. Jäckel, R. Schmid, H. Jones, T. Nakanaga and H. Takeo 215 (1997) 291
- A quantal entropy signature for the dynamics of pure states: Studies on some model problems, P. Sarkar, S. Adhikari and S.P. Bhattacharyya 215 (1997) 309
- Theoretical study of multiple high-order harmonic generation by intense ultrashort pulsed laser fields: A new generalized pseudospectral time-dependent method, X.-M. Tong and S.-I. Chu 217 (1997) 119
- Femtosecond quantum dynamics of photoassociation reactions: the exciplex formation of mercury, P. Backhaus and B. Schmidt 217 (1997) 131
- Phase-space localization and level spacing distributions for a driven rotor with mixed regular/chaotic dynamics, T. Gorin, H.J. Korsch and B. Mirbach 217 (1997) 145
- Ultracold atoms in modulated standing light waves, K. Drese and M. Holthaus 217 (1997) 201
- Photodissociation of Ar_2^+ in strong laser fields, P. Schwendner, F. Seyl and R. Schinke 217 (1997) 233
- Optimal pump-dump control, Y.J. Yan, J. Che and J.L. Krause 217 (1997) 297

- Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association, M.V. Korolkov, J. Manz and G.K. Paramonov 217 (1997) 341
- Reactions (including dissociation)*
- Experimental and theoretical study of the recombination reaction of FC(O)O radicals, A.E. Croce, C.J. Cobos and E. Castellano 211 (1996) 215
- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations, J.W. Boughton, S. Kristyan and M.C. Lin 214 (1997) 219
- The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory, A. Beghin and T. Stoecklin 215 (1997) 261
- On the determination of $D_0^0(\text{CaBr})$ from translational energy threshold measurements, M. Garay Salazar, J.M. Orea and A. González Ureña 216 (1997) 365
- Infrared bands of mass-selected carbon chains C_n ($n = 8-12$) and C_n^- ($n = 5-10, 12$) in neon matrices, P. Freivogel, M. Grutter, D. Forney and J.P. Maier 216 (1997) 401
- Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association, M.V. Korolkov, J. Manz and G.K. Paramonov 217 (1997) 341
- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Calculated thermodynamics of reactions involving $\text{NO}^+ \cdot \text{X}$ complexes (where $\text{X} = \text{H}_2\text{O}$, N_2 and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243
- Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257
- A three-body calculation for collision-induced dissociation, K. Sakai 220 (1997) 115
- Reaction dynamics of the $\text{Ca}(^1\text{D}_2, ^3\text{P}_j) + \text{CH}_3\text{I} \rightarrow \text{CaI}^* + \text{CH}_3$ system: chemiluminescence, energy disposal and product polarization, J.M. Orea, A. Laplaza, C.A. Rinaldi, G. Tardajos and A. González Ureña 220 (1997) 337
- A contribution to the theory of OD EPR of spin-correlated radical pairs, K.M. Salikhov, Y. Sakaguchi and H. Hayashi 220 (1997) 355
- gas phase*
- Experimental and theoretical study of the recombination reaction of FC(O)O radicals, A.E. Croce, C.J. Cobos and E. Castellano 211 (1996) 215
- Dynamics of the vibrational mode-specific proton transfer reaction $\text{NH}_3^+(\nu_1) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{NH}_4^+$: ab initio MO and classical trajectory studies, H. Tachikawa 211 (1996) 305
- Pressure effects on the $\text{Cl}_2(\text{D}'-\text{A}')$ transition at 258 nm, J.B. Nee and S. Hubinger 211 (1996) 403
- Comment on "energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm", S.W. North, T.J. Sears, G.E. Hall and T. Suzuki 211 (1996) 515
- Reaction path Hamiltonian analysis of the dynamics for $\text{Cl}^- + \text{CH}_3\text{Br} \rightarrow \text{ClCH}_3 + \text{Br}^-$ $\text{S}_\text{N}2$ nucleophilic substitution, H. Wang and W.L. Hase 212 (1996) 247
- A theoretical test of the pairwise energy model for reactive cross sections, J.-B. Song and E.A. Gislason 212 (1996) 259

- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Application of the pairwise energy model to various isotopic variations of the $H + H_2$ reaction, J.-B. Song and E.A. Gislason 214 (1997) 23
- The formation and dissociation of the dinitrogen pentoxide dication, C.S.S. O'Connor, N.C. Jones and S.D. Price 214 (1997) 131
- A Møller–Plesset perturbation theory and coupled-cluster study of the reaction enthalpies and barrier heights for the $FCO + H_2 \rightarrow HFCO + H$ abstraction reaction, J.S. Francisco 214 (1997) 213
- Theoretical study of the reaction of hydrogen with nitric acid: ab initio MO and TST/RRKM calculations, J.W. Boughton, S. Kristyan and M.C. Lin 214 (1997) 219
- On the $O_2(v') + O_2(v'')$ atmospheric reaction: a quasiclassical trajectory study, A.J.C. Varandas and W. Wang 215 (1997) 167
- The effect of middle range forces on the rate constant of a fast chemical reaction within adiabatic capture theory, A. Beghin and T. Stoecklin 215 (1997) 261
- Fine-structure dependence of the $Ar^*(^3P_{0,2}) + N_2(X)$ excitation transfer process, E.J.D. Vredenbregt, W.J.M. Rooyakkers, R.J.F. van Gerwen, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 259
- $Ar^*(^3P_2)/Kr^*(^3P_{0,2}) + N_2(X)$ excitation transfer collisions: final state rotational alignment, E.J.D. Vredenbregt, W.J.M. Rooyakkers, M.J.M. Vugts, P.J. van de Hurk and H.C.W. Beijerinck 216 (1997) 273
- Isotope effects on the rate constants for the processes $O_2 + O \rightarrow O + O_2$ and $O_2 + O + Ar \rightarrow O_3 + Ar$. On a modified ground-state potential energy surface for ozone, A. Gross and G.D. Billing 217 (1997) 1
- Theory of ultrafast laser control for state-selective dynamics of diatomic molecules in the ground electronic state: vibrational excitation, dissociation, spatial squeezing and association, M.V. Korolkov, J. Manz and G.K. Paramonov 217 (1997) 341
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
- Diatomics-in-molecules study of the ground and excited states of H_3^- , A.K. Belyaev and A.S. Tiukanov 220 (1997) 43
- Nonradiative processes and infrared emission in matrix isolated ND, N. Caspary, B.E. Wurfel, A.M. Smith and V.E. Bondybey 220 (1997) 241
- condensed phase*
- A Kramers reaction rate theory for electrochemical ion transfer reactions, M.T.M. Koper and W. Schmickler 211 (1996) 123
- Isotope effects in the photochemical formation of $HHgCH_3$ and $DHgCD_3$ in nitrogen and methane matrices, N. Legay-Sommaire and F. Legay 211 (1996) 367
- Dissociation constants of some substituted cinnamic acids in protic solvents: measurements by hyper-Rayleigh scattering and potentiometric techniques, P.C. Ray, N. Munichandriah and P.K. Das 211 (1996) 499
- Phenomenological interpretation of kinetics with time-dependent specific reaction rates, A. Plonka and A. Paszkiewicz 212 (1996) 1

- Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations, H. Sumi 212 (1996) 9
- Irreversible random transition theory as applied to rate processes in condensed media: Transient effects of constrained configuration rearrangements in complex systems, Yu.A. Berlin 212 (1996) 29
- An analytical study of the Berezhkovskii-Pollak-Zitserman theory of rate processes in the critical region. II. The critical coupling plane, S. Singh and G.W. Robinson 212 (1996) 125
- A temperature-dependent effective potential explains CO binding to myoglobin, N. Agmon and G.M. Sastry 212 (1996) 207
- Electronic charge density transfer along a constrained reaction path from a hydronium ion configuration into a hydrogen chemisorption state on Cu(100), An.M. Kuznetsov and W. Lorenz 214 (1997) 243
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part I: Manifold of stationarity conditions of hydrogen reaction emerging from dark to photoregimes of n-materials, and dark admittance evaluation, W. Lorenz, M. Handschuh and F. Bergmann 215 (1997) 139
- Charge transfer dynamics of electrochemical dark and photoprocesses on semiconductors. Part II: Fermi energy characteristics and photoadmittance functions, F. Bergmann, M. Handschuh and W. Lorenz 215 (1997) 157
- Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives, V.L. Vyazovkin and V.A. Tolkatchev 216 (1997) 135
- Phenomenological model for reaction kinetics coupled to a relaxing environment, Y.A. Berlin, A.L. Burin and S.F. Fischer 220 (1997) 25
- Quantum effects in adiabatic electrochemical electron-transfer reactions, M.T.M. Koper, J.-H. Mohr and W. Schmickler 220 (1997) 95
- Two-level system with noise: Blue's function approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 220 (1997) 125
- photochemical*
- Photophysics and photochemistry of I_2 (D, D') in rare gas clusters, K.L. Randall and D.J. Donaldson 211 (1996) 377
- Photophysics of 4-dimethylamino-4'-cyanostilbene and 4-azetidiny-4'-cyanostilbene. Time-resolved fluorescence and trans-cis photoisomerisation, Yu.V. Il'ichev, W. Kühnle and K.A. Zachariasse 211 (1996) 441
- Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique, F.F. Brazgun, V.A. Nadtochenko, I.V. Rubtsov and L.V. Lukin 211 (1996) 469
- Comment on "energy partitioning in photodissociation of methyl, ethyl, and *n*-propyl iodides at 304 nm", S.W. North, T.J. Sears, G.E. Hall and T. Suzuki 211 (1996) 515
- Remote ionization and recombination through the multichannel electron transfer, A.I. Burshtein and P.A. Frantsuzov 212 (1996) 137
- Photodissociation dynamics of $HN_3(DN_3) + h\nu \rightarrow H(D) + N_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385
- Ab initio determination of quasi-diabatic states for multiple reaction pathways, P. Cattaneo and M. Persico 214 (1997) 49
- A spectroscopic and photoisomerisation study of bromine dioxides in argon matrices, J. Kölm, A. Engdahl, O. Schrems and B. Nelander 214 (1997) 313

- Factors affecting adiabaticity in bimolecular photoinduced electron transfer reaction between anthracene derivatives and organic donors, X. Allonas and P. Jacques 215 (1997) 371
- Structure and selective visible photodissociation of the $O_3:Br_2$ and $O_3:BrCl$ complexes: an infrared matrix isolation and ab initio study, M. Bahou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 216 (1997) 105
- Optimal pump-dump control, Y.J. Yan, J. Che and J.L. Krause 217 (1997) 297
- Tunnelling*
- Control of tunneling reactions with an external field in a four-level system: A general Redfield approach, M. Morillo, C. Denk and R.I. Cukier 212 (1996) 157
- Time evolution of the rate constant for the tunneling reaction $H_2 + D \rightarrow H + HD$ in solid D_2-H_2 mixtures at very low temperature, T. Kumada, Y. Aratono and T. Miyazaki 212 (1996) 177
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- An ab initio treatment of the Norrish type-II process in pentane-2-one and the role of tunneling of hydrogen, V. Sreedhara Rao and A.K. Chandra 214 (1997) 103
- Tunnelling of the one-dimensional rotor NH_3D^+ in the NH_4ClO_4 and NH_4PF_6 lattices, H.G. Büttner, G.J. Kearley and B. Frick 214 (1997) 425
- The origin and temperature dependence of the single particle, methyl-group rotational potential in acetic acid, M.R. Johnson, M. Neumann, B. Nicolai, P. Smith and G.J. Kearley 215 (1997) 343
- Dynamical simulation of the driven spin-boson system: The influence of interblip correlations, M. Winterstetter and U. Weiss 217 (1997) 155
- Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations, M. Grifoni, L. Hartmann and P. Hänggi 217 (1997) 167
- Control of tunneling processes with an external field in a four-level system: an analytic approach, R.I. Cukier, C. Denk and M. Morillo 217 (1997) 179
- Dynamical resonance and tunneling in a driven system with periodic potential, E.M. Zanardi and J.M. Gomez Llorente 217 (1997) 221
- A theory of coherent control of reaction dynamics based on the optimization of a linear time-invariant system with complex variables, Y. Watanabe, H. Umeda, Y. Ohtsuki, H. Kono and Y. Fujimura 217 (1997) 317
- Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff 219 (1997) 119
- Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A. Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143
- Quantum effects in adiabatic electrochemical electron-transfer reactions, M.T.M. Koper, J.-H. Mohr and W. Schmickler 220 (1997) 95
- Line broadening in a polymer glass as investigated by stimulated photon echo spectroscopy: spectral diffusion versus heating effects, S.J. Zilker and D. Haarer 220 (1997) 167
- The tunneling frequencies of the isotopic forms of methane in rare-gas solids, D. Smith 220 (1997) 279
- Electron transfer*
- Solvent reorganization energy of electron transfer in weakly polar solvents, D.V. Matyushov 211 (1996) 47
- A Kramers reaction rate theory for electrochemical ion transfer reactions, M.T.M. Koper and W. Schmickler 211 (1996) 123
- The disperse kinetics of intercolumnar charge recombination in pulse-irradiated mesomorphic phthalocyanines, J.M. Warman, P.G. Schouten, G.H. Gelinck and M.P. de Haas 212 (1996) 183

- Competitive electron transfers in model triad systems: continuum model approach, T. Motylewski, J. Najbar and M. Tachiya 212 (1996) 193
- Spin-spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- A study of solvent dynamical effects on nonadiabatic electron transfer reaction rates, A. Samanta and S.K. Ghosh 214 (1997) 61
- Common features of various mechanisms of electron transfer across a 4,4'-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state, P. Karafiloglou 214 (1997) 171
- Electron attachment products of methylene chloride in solid argon: an experimental and quantum chemical IR spectroscopic study, A. Richter, H. Meyer, T. Kausche, T. Müller, W. Sporleder and A. Schweig 214 (1997) 321
- Double exchange in distorted trimeric mixed-valence clusters, M.I. Belinsky 215 (1997) 7
- Calculation of triplet-singlet transition efficiencies controlled by relative rotational diffusion of the two constituents of covalently linked radical pairs, K.M. Salikhov, J. Schlüpmann, M. Plato and K. Möbius 215 (1997) 23
- Single electron capture in low-energy $\text{Kr}^+ - \text{He}$ collisions, H. Martínez and J.M. Hernandez 215 (1997) 285
- Calculation of the solvent reorganization free energy in the dielectric cavity model, E.L. Mertz, E.D. German and A. M. Kuznetsov 215 (1997) 355
- Factors affecting adiabaticity in bimolecular photoinduced electron transfer reaction between anthracene derivatives and organic donors, X. Allonas and P. Jacques 215 (1997) 371
- Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy, J. Widengren, J. Dapprich and R. Rigler 216 (1997) 417
- Dynamical simulation of the driven spin-boson system: The influence of interblip correlations, M. Winterstetter and U. Weiss 217 (1997) 155
- Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations, M. Grifoni, L. Hartmann and P. Hänggi 217 (1997) 167
- Control of tunneling processes with an external field in a four-level system: an analytic approach, R.I. Cukier, C. Denk and M. Morillo 217 (1997) 179
- Dynamical resonance and tunneling in a driven system with periodic potential, E.M. Zanardi and J.M. Gomez Llorente 217 (1997) 221
- Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach, B. Wolfseder, L. Seidner, G. Stock and W. Domcke 217 (1997) 275
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331
- Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

- Quantum effects in adiabatic electrochemical electron-transfer reactions, M.T.M. Koper, J.-H. Mohr and W. Schmickler 220 (1997) 95
- The magnetic field influence on bridge-assisted electron transfer, E.G. Petrov, I.S. Tolokh, V.V. Gorbach and V. May 220 (1997) 249
- Positron annihilation*
- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures, A. Baranowski, K. Jerie and J. Gliński 214 (1997) 143
- Effects of CCl₄ on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions, M.F. Ferreira Marques, H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre 220 (1997) 233
- Ionization (including Rydberg states)*
- The dissociation energies of FeF, FeCl, and FeBr and their positive ions, C.W. Bauschlicher Jr. 211 (1996) 163
- Dynamics of geminate charge separation in liquid methylcyclohexane studied by the photoassisted ion pair separation technique, F.F. Brazgun, V.A. Nadtochenko, I.V. Rubtsov and L.V. Lukin 211 (1996) 469
- Ab initio study on the electronic structure of the $4^2\Sigma^+$ and $5^2\Sigma^+$ excited states of CO⁺, N. Honjou and E. Miyoshi 212 (1996) 363
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Experimental and theoretical study of the C_{1s} shakeup spectra from biphenyl and p-terphenyl, C. Enkvist, S. Lunell and S. Svensson 214 (1997) 123
- The formation and dissociation of the dinitrogen pentoxide dication, C.S.S. O'Connor, N.C. Jones and S.D. Price 214 (1997) 131
- Polarization propagator study of electronic excitation in key heterocyclic molecules I. Pyrrole, A.B. Trofimov and J. Schirmer 214 (1997) 153
- The molecular and electronic states of 1,2,4,5-tetrazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, D. Reed, A. Pollacchi, I.C. Walker, M.F. Guest and M.R.F. Siggel 214 (1997) 191
- The use of threshold photoelectron – fluorescence photon coincidence spectroscopy for the measurement of the radiative lifetimes of emitting states of CF₃X⁺ (X = F, H, Cl, Br) ions, H. Biehl, K.J. Boyle, D.M. Smith and R.P. Tuckett 214 (1997) 357
- Vacuum-UV fluorescence spectroscopy of CF₃X (X = F, H, Cl, Br) in the range 10–30 eV, H. Biehl, K.J. Boyle, R.P. Tuckett, H. Baumgärtel and H.W. Jochims 214 (1997) 367
- The van der Waals vibrational frequencies of the aniline–carbon monoxide complex in its S₁ state, J.-G. Jäckel, R. Schmid, H. Jones, T. Nakanaga and H. Takeo 215 (1997) 291
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases, M. Pulfer, C.-H. Hu and D.P. Chong 216 (1997) 91
- Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules, C.-H. Hu and D.P. Chong 216 (1997) 99
- Threshold photoelectron spectroscopy of SF₆, A.J. Yench, D.B. Thompson, A.J. Cormack, D.R. Cooper, M. Zubek, P. Bolognesi and G.C. King 216 (1997) 227

- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- Highly correlated QDPT-CI calculations of valence and core photoelectron spectra of Ne, G. Fronzoni and P. Decleva 220 (1997) 15
- The photoabsorption spectrum of vinylchloride (C_2H_3Cl) in the 8–12 eV range, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 207
- The He(I), threshold photoelectron and constant ion state spectroscopy of vinylchloride (C_2H_3Cl), R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 220 (1997) 217
- Molecular motion (including diffusive)*
- Monte Carlo simulation studies on the validity of the Gram–Charlier calculations of velocity distributions of Na^+ swarm in neon gas, P.P. Ong and M.-M. Li 211 (1996) 115
- Magnetic field dependent yield of geminate radical pair recombination in micelles. Effect of intraradical spin lattice relaxation, J.S. Jørgensen, J.B. Pedersen and A.I. Shushin 211 (1996) 235
- Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution, E.R. Middelhoeck, H. Zhang, J.W. Verhoeven and M. Glasbeek 211 (1996) 489
- Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations, H. Sumi 212 (1996) 9
- Recovering boundaries for partly diffusion-controlled reaction kinetics, N.J.B. Green, R.D. Spencer-Smith and A.G. Rickerby 212 (1996) 99
- Peculiarities of the diffusion of silver and sodium ions in phosphate glasses with a high content of Na_2O , V.M. Syutkin and V.A. Tolkmachev 212 (1996) 149
- Conformational flexibility of arginine-82 as source for the heterogeneous and pH-dependent kinetics of the primary proton transfer step in the bacteriorhodopsin photocycle: An electrostatic model, C. Scharnagl and S.F. Fischer 212 (1996) 231
- Reversible conformation change of free radicals in X-irradiated glutarimide single crystals studied by ENDOR, N.A. Salih, O.I. Eid, N.P. Benetis, M. Lindgren, A. Lund and E. Sagstuen 212 (1996) 409
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465
- Water residence times around copper plastocyanin: a molecular dynamics simulation approach, C. Rocchi, A.R. Bizzarri and S. Cannistraro 214 (1997) 261
- Influence of rotational diffusion on the electric field induced effect on the fluorescence spectrum of diluted solutions. I. Theory and numerical simulations, H. Reis and W. Baumann 214 (1997) 383
- Methyl radicals migration in glassy ethanol-1,2- d_5 at 90 K as studied by hydrogen atom abstraction from the additives, V.L. Vyazovkin and V.A. Tolkmachev 216 (1997) 135
- Stimulated emission processes and strong field effects in ultrashort pulse excitation of a predissociative molecule, H. Dietz, A. Materny and V. Engel 217 (1997) 249
- Optimal pump-dump control, Y.J. Yan, J. Che and J.L. Krause 217 (1997) 297
- Phenomenological model for reaction kinetics coupled to a relaxing environment, Y.A. Berlin, A.L. Burin and S.F. Fischer 220 (1997) 25
- The tunneling frequencies of the isotopic forms of methane in rare-gas solids, D. Smith 220 (1997) 279

Isotopic effects

- Isotope effects in the photochemical formation of HHgCH_3 and DHgCD_3 in nitrogen and methane matrices, N. Legay-Sommaire and F. Legay 211 (1996) 367
- Tunnelling of the one-dimensional rotor NH_3D^+ in the NH_4ClO_4 and NH_4PF_6 lattices, H.G. Büttner, G.J. Kearley and B. Frick 214 (1997) 425
- Inelastic neutron scattering studies of polyanilines and partially deuterated analogues, F. Fillaux, N. Leygue, R. Baddour-Hadjean, S. Parker, P. Colomban, A. Gruger, A. Régis and L.T. Yu 216 (1997) 281
- A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 , D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91

Fluctuations and noise

- Condition for fractional-power viscosity dependence of the average rate constant of solution reactions influenced by slow solvent fluctuations, H. Sumi 212 (1996) 9
- Dissipation and fluctuation for a randomly kicked particle: Normal and anomalous diffusion, E. Barkai and V. Fleurov 212 (1996) 69
- Comparison of the numerical matrix multiplication and quantum Monte Carlo simulations: calculation of spatial delocalization parameters, R.G. Schmidt, M.C. Böhm and J. Brickmann 215 (1997) 207
- A quantal entropy signature for the dynamics of pure states: Studies on some model problems, P. Sarkar, S. Adhikari and S.P. Bhattacharyya 215 (1997) 309
- Fast interactions between Rh6G and dGTP in water studied by fluorescence correlation spectroscopy, J. Widengren, J. Dapprich and R. Rigler 216 (1997) 417
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191

Collective motion and excitations

- Relaxation and trapping of excitons in J-aggregates of a thiocarbocynine dye, M.A. Drobizhev, M.N. Sapozhnikov, I.G. Scheblykin, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky 211 (1996) 455
- Irreversible random transition theory as applied to rate processes in condensed media: Transient effects of constrained configuration rearrangements in complex systems, Yu.A. Berlin 212 (1996) 29
- Vibron-mediated electronic relaxation in crystalline chlorine, D. Logan, C.A. Wight and V.A. Apkarian 217 (1997) 99

Surface effects and catalysis

- Stochastic wave packet vs. direct density matrix solution of Liouville–von Neumann equations for photodesorption problems, P. Saalfrank 211 (1996) 265
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Structures and potential energy surface of Faujasitic zeolite/water, J. Limtrakul, P. Treesukol, C. Ebner, R. Sansone and M. Probst 215 (1997) 77
- Disordered surfaces: a smoothed He–target scattering potential for metal atoms adsorbed on metal surfaces, G. Petrella, L. Cassidei and F. Ciriaco 216 (1997) 391
- “Free” nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43

Thermodynamic and transport properties

- Transport coefficients for NO^+ ions in helium gas: a test of the NO^+ –He interaction potential, L.A. Viehland, A.S. Dickinson and R.G.A.R. MacLagan 211 (1996) 1
- Maximum entropy imaging and quantum molecular timescale generalized Langevin equation theory, H.K. McDowell and A.M. Clogston 211 (1996) 91
- Monte Carlo simulation studies on the validity of the Gram–Charlier calculations of velocity distributions of Na^+ swarm in neon gas, P.P. Ong and M.-M. Li 211 (1996) 115
- The dissociation energies of FeF, FeCl, and FeBr and their positive ions, C.W. Bauschlicher Jr. 211 (1996) 163
- Universality of anomalous diffusion in extremely disordered systems, J.C. Dyre and J.M. Jacobsen 212 (1996) 61
- Dissipation and fluctuation for a randomly kicked particle: Normal and anomalous diffusion, E. Barkai and V. Fleurov 212 (1996) 69
- Reactions controlled by enhanced diffusion: Deterministic and stochastic approaches, G. Zumofen, J. Klafter and M.F. Shlesinger 212 (1996) 89
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Drift velocity of ions in lighter gases in electric and magnetic fields, L. Ferrari and A. Carbognani 215 (1997) 37
- Peculiarities of the enthalpy relaxation of a glassy crystal, O. Delcourt, M. Descamps, J. Even, M. Bertault and J.F. Willart 215 (1997) 51
- Effect of strong excitation of the CO_2 asymmetric mode on transport properties, A. Chikhaoui and E.V. Kustova 216 (1997) 297

Structure of solids and liquids

- Al,Si ordering in chabazites: A Monte Carlo study, M.C. Gordillo and C.P. Herrero 211 (1996) 81
- A QM/MM simulation method applied to the solution of Li^+ in liquid ammonia, T. Kerdcharoen, K.R. Liedl and B.M. Rode 211 (1996) 313
- Single molecule polarization spectroscopy: pentacene in p-terphenyl, F. Güttler, M. Croci, A. Renn and U.P. Wild 211 (1996) 421
- An ab initio perturbed ion study of structural properties of TiO_2 , SnO_2 and GeO_2 rutile lattices, A.C. Camargo, J.A. Igualada, A. Beltrán, R. Llusar, E. Longo and J. Andrés 212 (1996) 381
- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Positron annihilation in and compressibility of liquid water + tert-butyl alcohol mixtures, A. Baranowski, K. Jerie and J. Gliński 214 (1997) 143
- Orientational correlations in liquid carbon tetrabromide: a neutron diffraction and RMC study, I. Bakó, J.C. Dore and D.W. Huxley 216 (1997) 119
- Water structuring around complex solutes: theoretical modeling of α -D-glucopyranose, B. Leroux, H. Bizot, J.W. Brady and V. Tran 216 (1997) 349

- Effects of CCl_4 on positronium formation in pure isooctane and in AOT/water/isooctane microemulsions, M.F. Ferreira Marques, H.D. Burrows, M. da Graça Miguel, A.P. de Lima, C. Lopes Gil and G. Duplâtre 220 (1997) 233
- Structure and dynamics at the surface of a concentrated aqueous solution of CsF, J. Dietter and H. Morgner 220 (1997) 261
- Critical phenomena*
- An analytical study of the Berezhkovskii–Pollak–Zitserman theory of rate processes in the critical region. II. The critical coupling plane, S. Singh and G.W. Robinson 212 (1996) 125
- Temperature dependence of the density of an ionic micellar system near the critical point, A. Compostizo, C. Martín, R.G. Rubio and A. Crespo Colin 212 (1996) 301
- Electric permittivity in the one- and two-phase region of 1-nitropropane–hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483
- On the degrees of circularity for various kinds of polarized light in a nonpolar liquid mixture, D.J. Lee and K.-R. Kim 214 (1997) 183
- Phase transitions*
- The Neel point for spin-transition systems: toward a two-step transition, H. Bolvin 211 (1996) 101
- Solvent effects on sol–gel transition of alginate solutions by addition of cupric ions, H. Zheng, K. Jiang, Q. Zhang and J. Wang 211 (1996) 507
- A double origin proposed for the various Mössbauer spectra of biferrocenium salts: charge ordering and molecular bistability, F. Varret, J. Linares and K. Boukheddaden 212 (1996) 487
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357



Send for a Free Sample Copy!

Colloids and Surfaces B: Biointerfaces

An International Journal Devoted to Fundamental and Applied Research on Colloid and Interfacial Phenomena in Relation to Systems of Biological Origin

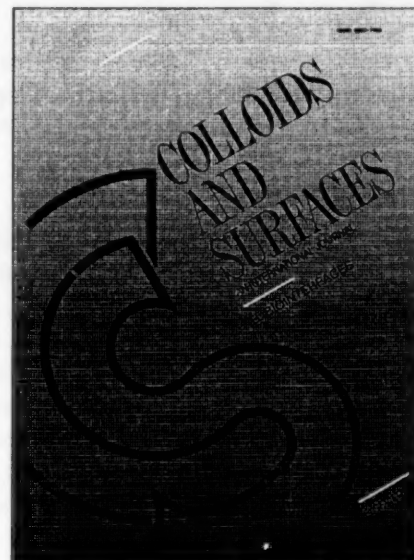
- Together with *Advances in Colloid and Interface Science*, this journal offers a complete coverage of the area
- Due to its editorial policy, adjustment of the journal contents continues to meet current market needs

Editors:

J.L. Brash, *McMaster University, Chemical Engineering Department, 1280 Main West Hamilton, Ont. L8S 4L7, Canada*, **H.J. Busscher**, *University of Groningen, Bloemsingel 10, 9712 KZ Groningen, The Netherlands* and **H. Ohshima**, *Faculty of Pharmaceutical Sciences, Science University of Tokyo, 12 Ichigaya Funagawara-machi, Shinjuku-ku, Tokyo 162, Japan*

AIMS AND SCOPE:

Colloids and Surfaces B: Biointerfaces is an international journal devoted to fundamental and applied research on colloid and interfacial phenomena in relation to systems of biological origin, having particular relevance to the medical, pharmaceutical, biotechnological, food and cosmetic fields. Papers on the use of experimental methods and their application to biological problems of an interfacial nature are also included.



For:

Colloid and Surface Chemists, Chemical Engineers, (Bio) Pharmaceutical, Cosmetic and Food Chemists, Physical Chemists, Polymer Chemists, Biological and Bioengineers, Organic Chemists, Microbiologists, Medicinal Chemists.

Colloids and Surfaces B: Biointerfaces

For more information, access <http://www.elsevier.nl/locate/colsurfb>

☐ Please send me a **FREE Sample Copy** including instructions to authors

Name: Initials:

Position: Title:

Institute/Company:

Department:

Address:

Post/Zip Code: City:

Country: Tel:

Fax: E-mail address:



New York

Tel: (+1) 212-633-3730
[Toll Free number for North American customers:
1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam

Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo

Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore

Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

Please quote the following code with all requests: **MD7**

Send for a Free Sample Copy!

Separation and Purification Technology

A merger of Separations Technology and Gas Separation & Purification

Editors:

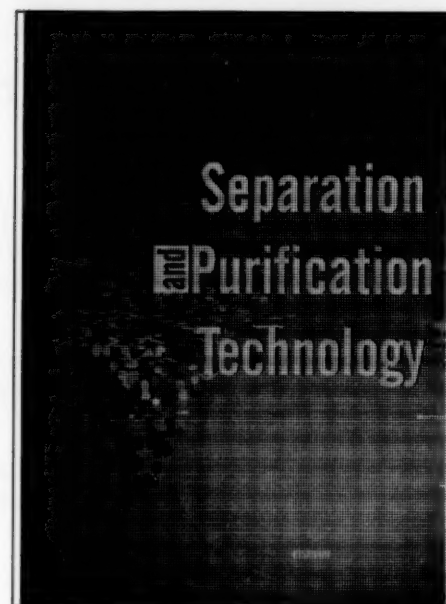
W. Baldus, Jaiserstrasse 51, D 82049 Pullach, Germany,
H. Strathmann, University of Twente, Faculty of Chemical Engineering, P.O. Box 217, 7500 AE Enschede, The Netherlands; Tel: (+31) 53 489 4611, Fax: (+31) 53 4892951/2950, E-mail: h.strathmann@ct.utwente.nl,

T. Takamatsu, 183 Iwakura-Hanazono, Sakyo, Kyoto 606, Japan; Fax: (+81) 75 781 4684, E-mail: tt-pse@po.ijnet.or.jp,

C. Tien, Department of Chemical Engineering and Materials Science, 320 Hinds Hall, Syracuse University, Syracuse, NY 13244-1190, USA; Tel: (+1) 315 443 1243, Fax: (+1) 315 443 4050/3351

AIMS AND SCOPE:

Separation and Purification Technology is a bimonthly international journal providing a comprehensive coverage of all aspects of separation and purification of homogeneous gaseous and liquid solutions and heterogeneous mixtures, such as emulsions or gas/solid, liquid/solid, and solid mixtures. *Separation and Purification Technology* welcomes in particular contributions focused on applications in the environmental protection industry, the recycling of valuable materials from industrial wastes, and the treatment of separation and purification problems in emerging technologies including energy storage and conversion systems, raw material and renewable energy exploitation, biotechnology and chemical or petrochemical processing.



For:
Membrane Technologists, Chemical Engineers and Separation Scientists.

Separation and Purification Technology

For more information, access <http://www.elsevier.nl/locate/seppur>

☐ Please send me a **FREE Sample Copy** including instructions to authors

Name: Initials:

Position: Title:

Institute/Company:

Department:

Address:

Post/Zip Code: City:

Country: Tel:

Fax: E-mail address:



New York
Tel: (+1) 212-633-3730
[Toll Free number for North American customers: 1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam
Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo
Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore
Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

Please quote the following code with all requests: MD7

Chemical Physics

(continued from inside front cover)

Submission of papers: All papers should be submitted in *quadruplicate* to one of the editors.

Electronic manuscripts: Electronic manuscripts have the advantage that there is no need for the rekeying of text, thereby avoiding the possibility of introducing errors and resulting in reliable and fast delivery of proofs.

For the initial submission of manuscripts for consideration, hardcopies are sufficient. For the processing of *accepted papers*, electronic versions are preferred. After *final acceptance*, your disk plus one final and exactly matching printed version should be submitted together. Double density (DD) or high density (HD) diskettes (3.5 or 5.25 inch) are acceptable. It is important that the file saved is in the native format of the wordprocessor program used. Label the disk with the name of the computer and wordprocessing package used, your name, and the name of the file on the disk.

Important: please adhere to instructions to authors, to be found on the last pages of each volume. The instructions can also be found on the World Wide Web: access under <http://www.elsevier.nl> or <http://www.elsevier.com>.

Proofs: Authors will receive proofs, which they are requested to correct and return as soon as possible. No new material may be inserted in the text at the time of proofreading.

All questions arising after acceptance of the manuscript, especially those relating to proofs, should be directed to *Chemical Physics*, Elsevier Science B.V., P.O. Box 2759, 1000 CT Amsterdam, The Netherlands. Tel. (+31-20)4852-800, Fax (+31-20)4852-775, E-mail: e.hovens@elsevier.nl

Authors in Japan please note: Upon request, Elsevier Science Japan will provide authors with a list of people who can check and improve the English of their paper (*before submission*). Please contact our Tokyo office: Elsevier Science Japan, 1-9-15 Higashi-Azabu, Minato-ku, Tokyo 106, Tel. (03)-5561-5032; Fax (03)-5561-5045.

Chemical Physics has no page charges.

Publication information. *Chemical Physics* (ISSN 0301-0104). For 1997 volumes 214–226 are scheduled for publication. Subscription prices are available upon request from the publisher. Subscriptions are accepted on a prepaid basis only and are entered on a calendar year basis. Issues are sent by surface mail except to the following countries where air delivery via SAL is ensured: Argentina, Australia, Brazil, Canada, Hong Kong, India, Israel, Japan, Malaysia, Mexico, New Zealand, Pakistan, PR China, Singapore, South Africa, South Korea, Taiwan, Thailand, USA. For all other countries airmail rates are available upon request. Claims for missing issues must be made within six months of our publication (mailing) date.

Orders, claims, and product enquiries: please contact the Customer Support Department at the Regional Sales Office nearest to you:

New York, Elsevier Science, P.O. Box 945, New York, NY 10159-0945, USA. Tel: (+1) 212-633-3730, [Toll free number for North American customers: 1-888-4ES-INFO (437-4636)], Fax: (+1)212-633-3680, E-mail: usinfo-f@elsevier.com

Amsterdam, Elsevier Science, P.O. Box 211, 1000 AE Amsterdam, The Netherlands. Tel: (+31)20-4853757, Fax: (+31)20-4853432, E-mail: nlinfo-f@elsevier.nl

Tokyo, Elsevier Science, 9-15 Higashi-Azabu 1-chome, Minato-ku, Tokyo 106, Japan. Tel: (+81)3-5561-5033, Fax: (+81)3-5561-5047, E-mail: kyf04035@niftyserve.or.jp

Singapore, Elsevier Science, No. 1 Temasek Avenue, #17-01 Millenia Tower, Singapore 039192. Tel: (+65)434-3727, Fax: (+65)337-2230, E-mail: asiainfo@elsevier.com.sg

Advertising information: Advertising orders and enquiries may be sent to: **International:** Elsevier Science, Advertising Department, The Boulevard, Langford Lane, Kidlington, Oxford, OX5 1GB, UK. Tel. (+44)(0)1865 843565, Fax (+44)(0)1865 843976. **USA and Canada:** Weston Media Associates, Dan Lipner, P.O. Box 1110, Greens Farms, CT 06436-1110, USA, Tel. (+1)(203)261-2500; Fax (+1)(203)261-0101. **Japan:** Elsevier Science Japan, Marketing Services, 1-9-15 Higashi-Azabu, Minato-ku, Tokyo 106, Japan; Tel.: (+81)-3-5561-5033, Fax (+81)-3-5561-5047.

US mailing notice. *Chemical Physics* (ISSN 0301-0104) is published semi-monthly by Elsevier Science NL (P.O. Box 211, 1000 AE Amsterdam, The Netherlands). Annual subscription price in the USA US\$ 4735.00 (valid in North, Central and South America), including air speed delivery. Periodicals postage paid at Jamaica, NY 11431.

USA POSTMASTERS: Send address changes to: Chemical Physics, Publications Expediting Inc., 200 Meacham Avenue, Elmont, NY 11003. Airfreight and mailing in the USA by Publication Expediting Inc., 200 Meacham Avenue, Elmont, NY 11003..

⊗ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

PRINTED IN THE NETHERLANDS

Send for a Free Sample Copy!

Thermochimica Acta

An International Journal Concerned with All Aspects of Thermoanalytical and Calorimetric Methods and their Application to Experimental Chemistry, Physics, Biology and Engineering

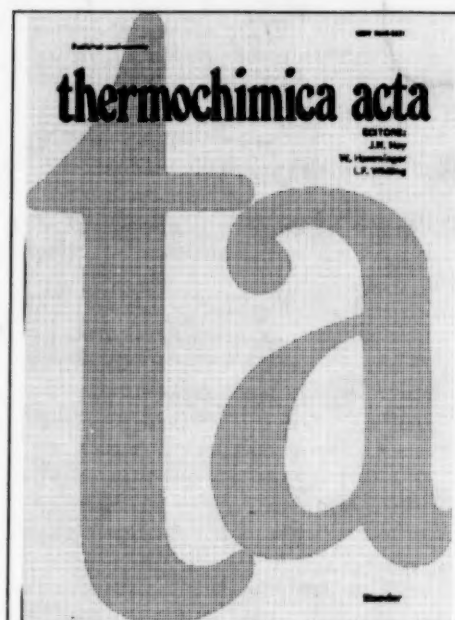
- Depth in methodology
- Breadth in applications
- Covers > 35% of papers in the field
- Free contents alerting service via e-mail

Editors:

J.L. Ford, School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK,
L.D. Hansen, Department of Chemistry and Biochemistry, C100 BNSN, Brigham Young University, Provo, UT 84602-5700, USA, **J.N. Hay**, School of Chemistry, University of Birmingham, Birmingham B15 2TT, UK, **W. Hemminger**, Physikalisch-Technische Bundesanstalt, Postfach 33 45, 38023 Braunschweig, (Bundesallee 100, 38116 Braunschweig), Germany and **L.F. Whiting**, Analytical Sciences, Dow Chemical Co., B-1216 Building, Freeport, TX 77541, USA

AIMS AND SCOPE:

Thermochimica Acta publishes original research contributions relating to fundamental and applied research in the fields of thermal analysis and calorimetry. These methods apply to problems in the physical and biomedical sciences and engineering. Specific areas of research include instrumentation, new and improved methods of investigation, analysis and interpretation of research data, and applications in industry.



For:

Principally Chemists but also Physicists, Biologists, Metallurgists and Mineralogists interested in the techniques and applications of thermal analysis and thermochemistry.

Thermochimica Acta
<http://www.elsevier.nl/locate/tca>

☐ Please send me a **FREE Sample Copy** including instructions to authors

Name: Initials:

Position: Title:

Institute/Company:

Department:

Address:

Post/Zip Code: City:

Country: Tel:

Fax: E-mail address:



New York
Tel: (+1) 212-633-3730
[Toll Free number for North American customers:
1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam
Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo
Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore
Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

Please quote the following code with all requests: MD7

12/97



0301-0104(199708)211/220;1-2

